

## Chemical Safety Data Sheet MSDS / SDS

## Xanthohumol

Revision Date:2024-11-02 Revision Number:1

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

## Product identifier

Product name : Xanthohumol  
CBnumber : CB5128899  
CAS : 6754-58-1  
Synonyms : XANTHOTHUMOL,(E)-1-[2,4-Dihydroxy-6-Methoxy-3-(3-Methylbut-2-Enyl)phenyl]-3-(4-Hydroxyphenyl)prop-2-En-1-One

## 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

## GHS Label elements, including precautionary statements

Symbol(GHS)



Signal word

Warning

## Precautionary statements

P273 Avoid release to the environment.  
P280 Wear protective gloves/protective clothing/eye protection/face protection.

## Hazard statements

H317 May cause an allergic skin reaction  
H400 Very toxic to aquatic life

## SECTION 3: Composition/information on ingredients

## Substance

Product name	: Xanthohumol
Synonyms	: XANTHOTHUMOL,(E)-1-[2,4-Dihydroxy-6-Methoxy-3-(3-Methylbut-2-Enyl)phenyl]-3-(4-Hydroxyphenyl)prop-2-En-1-One
CAS	: 6754-58-1
MF	: C <sub>21</sub> H <sub>22</sub> O <sub>5</sub>
MW	: 354.4

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## SECTION 4: First aid measures

### **Most important symptoms and effects, both acute and delayed**

The most important known symptoms and effects are described in the labelling (see section 2.2) and/or in section 11

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

No data available

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## SECTION 5: Firefighting measures

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

Carbon oxides

### **Advice for firefighters**

No data available

### **Further information**

No data available

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## SECTION 6: Accidental release measures

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

For personal protection see section 8.

### **Environmental precautions**

No data available

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

No data available

### **Reference to other sections**

For disposal see section 13.

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## SECTION 7: Handling and storage

## Precautions for safe handling

For precautions see section 2.2.

## Conditions for safe storage, including any incompatibilities

Recommended storage temperature 2 - 8 °C

## Specific end use(s)

Apart from the uses mentioned in section 1.2 no other specific uses are stipulated

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# SECTION 8: Exposure controls/personal protection

## control parameter

### Hazard composition and occupational exposure limits

Does not contain substances with occupational exposure limits.

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# SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

Appearance	powder
Odour	No data available
Odour Threshold	No data available
pH	No data available
Melting point/freezing point	Melting point: 172 °C
Initial boiling point and boiling range	576.5±50.0 °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
Vapour pressure	No data available
Vapour density	No data available
Relative density	No data available
Water solubility	ethanol: soluble10mg/mL
Partition coefficient: n-octanol/water	No data available
Autoignition temperature	No data available
Decomposition temperature	No data available
Viscosity	No data available
Explosive properties	No data available
Oxidizing properties	No data available

## Other safety information

No data available

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## SECTION 10: Stability and reactivity

### **Reactivity**

No data available

### **Chemical stability**

No data available

### **Possibility of hazardous reactions**

No data available

### **Conditions to avoid**

No data available

### **Incompatible materials**

Strong oxidizing agents

### **Hazardous decomposition products**

Hazardous decomposition products formed under fire conditions. - Carbon oxides Other decomposition products - No data available

In the event of fire: see section 5

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## SECTION 11: Toxicological information

### **Information on toxicological effects**

#### **Acute toxicity**

No data available

#### **Skin corrosion/irritation**

No data available

#### **Serious eye damage/eye irritation**

No data available

#### **Respiratory or skin sensitisation**

No data available

#### **Germ cell mutagenicity**

No data available

#### **Carcinogenicity**

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

#### **Reproductive toxicity**

No data available

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

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

**Additional Information**

RTECS: Not available

To the best of our knowledge, the chemical, physical, and toxicological properties have not been thoroughly investigated.

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## SECTION 12: Ecological information

**Toxicity**

No data available

**Persistence and degradability**

No data available

**Bioaccumulative potential**

No data available

**Mobility in soil**

No data available

**Results of PBT and vPvB assessment**

This substance/mixture contains no components considered to be either persistent, bioaccumulative and toxic (PBT), or very persistent and very bioaccumulative (vPvB) at levels of 0.1% or higher.

**Other adverse effects**

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## SECTION 13: Disposal considerations

**Waste treatment methods**

**Product**

No data available

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## SECTION 14: Transport information

**UN number**

ADR/RID: 3077 IMDG: 3077 IATA: 3077

**UN proper shipping name**

ADR/RID: ENVIRONMENTALLY HAZARDOUS SUBSTANCE, SOLID, N.O.S. (Xanthohumol) IMDG: ENVIRONMENTALLY HAZARDOUS

SUBSTANCE, SOLID, N.O.S. (Xanthohumol)

IATA: Environmentally hazardous substance, solid, n.o.s. (Xanthohumol)

### **Transport hazard class(es)**

ADR/RID: 9 IMDG: 9 IATA: 9

### **Packaging group**

ADR/RID: III IMDG: III IATA: III

### **Environmental hazards**

ADR/RID: yes IMDG Marine pollutant: yes IATA: yes

### **Special precautions for user**

### **Further information**

EHS-Mark required (ADR 2.2.9.1.10, IMDG code 2.10.3) for single packagings and combination packagings containing inner packagings with Dangerous Goods > 5L for liquids or > 5kg for solids.

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## SECTION 15: Regulatory information

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

#### **Regulations on the Safety Management of Hazardous Chemicals**

China Catalog of Hazardous chemicals 2015:Not Listed. website: <https://www.mem.gov.cn/>

#### **Measures for Environmental Management of New Chemical Substances**

Vietnam National Chemical Inventory:Listed. website: <https://chemicaldata.gov.vn/>

Chinese Chemical Inventory of Existing Chemical Substances (China IECSC):Not Listed. website: <https://www.mee.gov.cn/>

EC Inventory:Not Listed.

European Inventory of Existing Commercial Chemical Substances (EINECS):Not Listed. website: <https://echa.europa.eu/>

Korea Existing Chemicals List (KECL):Not Listed. website: <http://ncis.nier.go.kr>

New Zealand Inventory of Chemicals (NZIoC):Not Listed. website: <https://www.epa.govt.nz/>

Philippines Inventory of Chemicals and Chemical Substances (PICCS):Not Listed. website: <https://emb.gov.ph/>

United States Toxic Substances Control Act (TSCA) Inventory:Not Listed. website: <https://www.epa.gov/>

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## SECTION 16: Other information

### **Abbreviations and acronyms**

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

CAS: Chemical Abstracts Service

EC50: Effective Concentration 50%

IATA: International Air Transportation Association

IMDG: International Maritime Dangerous Goods

LC50: Lethal Concentration 50%

LD50: Lethal Dose 50%

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

STEL: Short term exposure limit

TWA: Time Weighted Average

## References

- 【1】 CAMEO Chemicals, website: <http://cameochemicals.noaa.gov/search/simple>
- 【2】 ChemIDplus, website: <http://chem.sis.nlm.nih.gov/chemidplus/chemidlite.jsp>
- 【3】 ECHA - European Chemicals Agency, website: <https://echa.europa.eu/>
- 【4】 eChemPortal - The Global Portal to Information on Chemical Substances by OECD, website:  
[http://www.echemportal.org/echemportal/index?pageID=0&request\\_locale=en](http://www.echemportal.org/echemportal/index?pageID=0&request_locale=en)
- 【5】 ERG - Emergency Response Guidebook by U.S. Department of Transportation, website: <http://www.phmsa.dot.gov/hazmat/library/erg>
- 【6】 Germany GESTIS-database on hazard substance, website: <http://www.dguv.de/ifa/gestis/gestis-stoffdatenbank/index-2.jsp>
- 【7】 HSDB - Hazardous Substances Data Bank, website: <https://toxnet.nlm.nih.gov/newtoxnet/hsdb.htm>
- 【8】 IARC - International Agency for Research on Cancer, website: <http://www.iarc.fr/>
- 【9】 IPCS - The International Chemical Safety Cards (ICSC), website: <http://www.ilo.org/dyn/icsc/showcard.home>
- 【10】 Sigma-Aldrich, website: <https://www.sigmaaldrich.com/>

### 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.