

## Chemical Safety Data Sheet MSDS / SDS

**(E)-2-methoxy-4-(prop-1-enyl)phenol**Revision Date:2023-05-06 Revision Number:1

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

Product name : (E)-2-methoxy-4-(prop-1-enyl)phenol  
CBnumber : CB9912748  
CAS : 5932-68-3  
EINECS Number : 227-678-2  
Synonyms : Phenol, 2-methoxy-4-(1-propenyl)-, (E)-, (E)-isoeugenol

**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

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**SECTION 2: Hazards identification****Classification of the substance or mixture**

Skin sensitization, Sub-category 1A

**Label elements****Pictogram(s)**

□

Signal word : Warning

**Hazard statement(s)**

H315 Causes skin irritation

H317 May cause an allergic skin reaction

H319 Causes serious eye irritation

H335 May cause respiratory irritation

**Precautionary statement(s)**

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

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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P333+P313 IF SKIN irritation or rash occurs: Get medical advice/attention.

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

#### **Prevention**

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/...

#### **Response**

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

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## SECTION 3: Composition/information on ingredients

### **Substance**

Product name	: (E)-2-methoxy-4-(prop-1-enyl)phenol
Synonyms	: Phenol, 2-methoxy-4-(1-propenyl)-, (E)-, (E)-isoeugenol
CAS	: 5932-68-3
EC number	: 227-678-2
MF	: C10H12O2
MW	: 164.2

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## SECTION 4: First aid measures

### **Description of first aid measures**

#### **If inhaled**

Move the victim into fresh air. If breathing is difficult, give oxygen. If not breathing, give artificial respiration and consult a doctor immediately.

Do not use mouth to mouth resuscitation if the victim ingested or inhaled the chemical.

#### **Following skin contact**

Take off contaminated clothing immediately. Wash off with soap and plenty of water. Consult a doctor.

#### **Following eye contact**

Rinse with pure water for at least 15 minutes. Consult a doctor.

#### **Following ingestion**

Rinse mouth with water. Do not induce vomiting. Never give anything by mouth to an unconscious person. Call a doctor or Poison Control Center immediately.

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

no data available

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

Immediate first aid: Ensure that adequate decontamination has been carried out. If patient is not breathing, start artificial respiration, preferably with a demand-valve resuscitator, bag-valve-mask device, or pocket mask, as trained. Perform CPR as necessary. Immediately flush contaminated eyes with gently flowing water. Do not induce vomiting. If vomiting occurs, lean patient forward or place on left side (head-down position, if possible) to maintain an open airway and prevent aspiration. Keep patient quiet and maintain normal body temperature. Obtain medical attention. Phenols and related compounds

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## SECTION 5: Firefighting measures

### **Extinguishing media**

This compound is not very flammable but any fire involving this compound may produce dangerous vapors. You should evacuate the area. All firefighters should wear full-body protective clothing and use self-contained breathing apparatuses. You should extinguish any fires involving this chemical with a dry chemical, carbon dioxide, foam, or halon extinguisher. (NTP, 1992)

### **Specific Hazards Arising from the Chemical**

This chemical is combustible. (NTP, 1992)

### **Advice for firefighters**

Wear self-contained breathing apparatus for firefighting if necessary.

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## SECTION 6: Accidental release measures

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

Avoid dust formation. Avoid breathing mist, gas or vapours. Avoid contacting with skin and eye. Use personal protective equipment. Wear chemical impermeable gloves. Ensure adequate ventilation. Remove all sources of ignition. Evacuate personnel to safe areas. Keep people away from and upwind of spill/leak.

### **Environmental precautions**

Prevent further spillage or leakage if it is safe to do so. Do not let the chemical enter drains. Discharge into the environment must be avoided.

### **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.

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## SECTION 7: Handling and storage

## Precautions for safe handling

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

Store the container tightly closed in a dry, cool and well-ventilated place. Store apart from foodstuff containers or incompatible materials.

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# 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 tightly fitting safety goggles with side-shields conforming to EN 166(EU) or NIOSH (US).

### Skin protection

Wear fire/flamm resistant and impervious clothing. Handle with gloves. Gloves must be inspected prior to use. Wash and dry hands. The selected protective gloves have to satisfy the specifications of EU Directive 89/686/EEC and the standard EN 374 derived from it.

### Respiratory protection

If the exposure limits are exceeded, irritation or other symptoms are experienced, use a full-face respirator.

### Thermal hazards

no data available

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# SECTION 9: Physical and chemical properties

## Information on basic physicochemical properties

Physical state	Liquid. Slightly viscous.
Colour	Pale yellow.
Odour	Spice-clove odor
Melting point/freezing point	27.3 °C. Atm. press.:981 mBar. Remarks:Accuracy +/- 2°C.
Boiling point or initial boiling point and boiling range	Remarks:Boiling temperature of test substance was not determinable, as the test substance decomposed at temperatures above approximately 130°C, under normal atmospheric pressure, before boiling.
Flammability	no data available

Lower and upper explosion	no data available
limit/flammability limit	
Flash point	132 °C. Atm. press.:981 mBar.
Auto-ignition temperature	380 °C. Atm. press.:98 508 - 99 608 Pa.
Decomposition temperature	no data available
pH	no data available
Kinematic viscosity	7.476 centipoise at 20 deg C
Solubility	Slightly soluble (NTP, 1992)
Partition coefficient n-octanol/water	log Pow = 2.1. Temperature:25 °C. Remarks:Trans isomer.
Vapour pressure	1 Pa. Temperature:25 °C. Remarks:Interpolated.
Density and/or relative density	1.083. Temperature:25 °C.
Relative vapour density	no data available
Particle characteristics	no data available

## SECTION 10: Stability and reactivity

### Reactivity

Slightly water soluble (NTP, 1992).

### Chemical stability

no data available

### Possibility of hazardous reactions

no data available

### 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 oral 1560 mg/kg
- Inhalation: no data available
- Dermal: no data available

### 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**

no data available

**Reproductive toxicity**

no data available

**STOT-single exposure**

no data available

**STOT-repeated exposure**

no data available

**Aspiration hazard**

no data available

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## SECTION 12: Ecological information

**Toxicity**

Toxicity to fish: LC50 - *Danio rerio*, *Oncorhynchus mykiss*, *Lepomis macrochirus*, *Pimephales promelas*, *Oryzias latipes*, *Leuciscus idus* - 3.6 mg/L - 96 h.

Toxicity to daphnia and other aquatic invertebrates: EC50 - *Daphnia magna*, *Daphnia pulex* - 3 mg/L - 48 h.

Toxicity to algae: EC50 - *Pseudokirchneriella subcapitata*, *Desmodesmus subspicatus*, *Scenedesmus quadricauda* - 5.6 mg/L - 72 h.

Toxicity to microorganisms: no data available

**Persistence and degradability**

AEROBIC: Isoeugenol, at a concentration of 100 mg/L, was found to be readily biodegradable using a Manometric Respirometry Test (OECD Guideline 301F) in which isoeugenol reached 79% biodegradation after 28 days(1); the biodegradation started on day 2 and reached 79% at the end of the 10-day window period(1).

**Bioaccumulative potential**

An estimated BCF of 47 was calculated in fish for isoeugenol(SRC), using a log Kow of 3.04(1) and a regression-derived equation(2). According to a classification scheme(3), this BCF suggests the potential for bioconcentration in aquatic organisms is moderate(SRC).

**Mobility in soil**

Using a structure estimation method based on molecular connectivity indices(1), the Koc of isoeugenol can be estimated to be 680(SRC). According to a classification scheme(2), this estimated Koc value suggests that isoeugenol is expected to have low mobility in soil.

### **Other adverse effects**

no data available

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## **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.

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## **SECTION 14: Transport information**

### **UN Number**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **UN Proper Shipping Name**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

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

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (For reference only, please check.)

### **Packing group, if applicable**

ADR/RID: Not dangerous goods. (For reference only, please check.)

IMDG: Not dangerous goods. (For reference only, please check.)

IATA: Not dangerous goods. (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

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## 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

Not Listed.

#### China Catalog of Hazardous chemicals 2015

Not Listed.

#### New Zealand Inventory of Chemicals (NZIoC)

Not Listed.

#### PICCS

Listed.

#### Vietnam National Chemical Inventory

Not Listed.

#### IECSC

Listed.

#### Korea Existing Chemicals List (KECL)

Not Listed.

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## 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](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:

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.