

# SAFETY DATA SHEET

according to Regulation (EC) No. 1907/2006

Version 9.0

Revision Date 14.08.2024

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GENERIC EU MSDS - NO COUNTRY SPECIFIC DATA - NO OEL DATA

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

### 1.1 Product identifiers

Product name : Guaiacol Impurity E

Product Number : PHR2475

Brand : Sigma-Aldrich

REACH No. : 01-2119969268-21-XXXX

CAS-No. : 93-58-3

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

Identified uses : Laboratory chemicals, Manufacture of substances

### 1.3

### 1.4 Emergency telephone

Emergency Phone # : 000 800 1007 141 (CHEMTREC)

## SECTION 2: Hazards identification

### 2.1 Classification of the substance or mixture

Acute toxicity, (Category 4) H302: Harmful if swallowed.

Reproductive toxicity, (Category 2) H361d: Suspected of damaging the unborn child.

### 2.2 Label elements

#### Labelling according Regulation (EC) No 1272/2008

Pictogram

Signal Word : Warning

Hazard Statements

H302 Harmful if swallowed.

H361d Suspected of damaging the unborn child.

|                                |                                                                               |
|--------------------------------|-------------------------------------------------------------------------------|
| Precautionary Statements       |                                                                               |
| P202                           | Do not handle until all safety precautions have been read and understood.     |
| P264                           | Wash skin thoroughly after handling.                                          |
| P280                           | Wear protective gloves/ protective clothing/ eye protection/ face protection. |
| P301 + P312                    | IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell.                |
| P308 + P313                    | IF exposed or concerned: Get medical advice/ attention.                       |
| P405                           | Store locked up.                                                              |
| Supplemental Hazard Statements | none                                                                          |

### Reduced Labeling (<= 125 ml)

Pictogram

|                                |                                                                               |
|--------------------------------|-------------------------------------------------------------------------------|
| Signal Word                    | Warning                                                                       |
| Hazard Statements              |                                                                               |
| H361d                          | Suspected of damaging the unborn child.                                       |
| Precautionary Statements       |                                                                               |
| P202                           | Do not handle until all safety precautions have been read and understood.     |
| P280                           | Wear protective gloves/ protective clothing/ eye protection/ face protection. |
| P308 + P313                    | IF exposed or concerned: Get medical advice/ attention.                       |
| P405                           | Store locked up.                                                              |
| Supplemental Hazard Statements | none                                                                          |

### 2.3 Other hazards

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.

Ecological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

Toxicological information:

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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## SECTION 3: Composition/information on ingredients

### 3.1 Substances

|                  |                                                    |
|------------------|----------------------------------------------------|
| Formula          | : C <sub>6</sub> H <sub>5</sub> COOCH <sub>3</sub> |
| Molecular weight | : 136,15 g/mol                                     |
| CAS-No.          | : 93-58-3                                          |
| EC-No.           | : 202-259-7                                        |

| Component              |           | Classification                        | Concentration |
|------------------------|-----------|---------------------------------------|---------------|
| <b>Methyl benzoate</b> |           |                                       |               |
| CAS-No.                | 93-58-3   | Acute Tox. 4; Repr. 2;<br>H302, H361d | <= 100 %      |
| EC-No.                 | 202-259-7 |                                       |               |

For the full text of the H-Statements mentioned in this Section, see Section 16.

## SECTION 4: First aid measures

### 4.1 Description of first-aid measures

#### General advice

Show this material safety data sheet to the doctor in attendance.

#### If inhaled

After inhalation: fresh air. Call in physician.

#### In case of skin contact

In case of skin contact: Take off immediately all contaminated clothing. Rinse skin with water/ shower. Consult a physician.

#### In case of eye contact

After eye contact: rinse out with plenty of water. Call in ophthalmologist. Remove contact lenses.

#### If swallowed

After swallowing: immediately make victim drink water (two glasses at most). Consult 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 2.2) and/or in section 11

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

No data available

## SECTION 5: Firefighting measures

### 5.1 Extinguishing media

#### Suitable extinguishing media

Water Foam Carbon dioxide (CO<sub>2</sub>) Dry powder

#### Unsuitable extinguishing media

For this substance/mixture no limitations of extinguishing agents are given.

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

Carbon oxides

Combustible.

Vapors are heavier than air and may spread along floors.

Forms explosive mixtures with air on intense heating.

Development of hazardous combustion gases or vapours possible in the event of fire.

### 5.3 Advice for firefighters

Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

## 5.4 Further information

Remove container from danger zone and cool with water. Prevent fire extinguishing water from contaminating surface water or the ground water system.

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## SECTION 6: Accidental release measures

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

Advice for non-emergency personnel: Do not breathe vapors, aerosols. Avoid substance contact. Ensure adequate ventilation. Keep away from heat and sources of ignition. Evacuate the danger area, observe emergency procedures, consult an expert. For personal protection see section 8.

### 6.2 Environmental precautions

Do not let product enter drains.

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

Cover drains. Collect, bind, and pump off spills. Observe possible material restrictions (see sections 7 and 10). Take up with liquid-absorbent material (e.g. Chemizorb® ). Dispose of properly. Clean up affected area.

### 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

#### Advice on protection against fire and explosion

Keep away from open flames, hot surfaces and sources of ignition. Take precautionary measures against static discharge.

#### Hygiene measures

Change contaminated clothing. Preventive skin protection recommended. Wash hands after working with substance.

For precautions see section 2.2.

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

#### Storage conditions

Tightly closed. Keep locked up or in an area accessible only to qualified or authorized persons.

#### Storage class

Storage class (TRGS 510): 10: Combustible liquids

### 7.3 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**

### **8.1 Control parameters**

#### **Ingredients with workplace control parameters**

### **8.2 Exposure controls**

#### **Personal protective equipment**

##### **Eye/face protection**

Use equipment for eye protection tested and approved under appropriate government standards such as NIOSH (US) or EN 166(EU). Safety glasses

##### **Skin protection**

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Full contact

Material: butyl-rubber

Minimum layer thickness: 0,7 mm

Break through time: 480 min

Material tested: Butoject® (KCL 898)

This recommendation applies only to the product stated in the safety data sheet, supplied by us and for the designated use. When dissolving in or mixing with other substances and under conditions deviating from those stated in EN 16523-1 please contact the supplier of CE-approved gloves (e.g. KCL GmbH, D-36124 Eichenzell, Internet: [www.kcl.de](http://www.kcl.de)).

Splash contact

Material: Nitrile rubber

Minimum layer thickness: 0,4 mm

Break through time: 10 min

Material tested: Camatril® (KCL 730 / Aldrich Z677442, Size M)

##### **Body Protection**

protective clothing

##### **Respiratory protection**

Recommended Filter type: Filter A (acc. to DIN 3181) for vapours of organic compounds

The entrepreneur has to ensure that maintenance, cleaning and testing of respiratory protective devices are carried out according to the instructions of the producer. These measures have to be properly documented.

##### **Control of environmental exposure**

Do not let product enter drains.

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## **SECTION 9: Physical and chemical properties**

### **9.1 Information on basic physical and chemical properties**

- |                   |               |
|-------------------|---------------|
| a) Physical state | clear, liquid |
| b) Color          | colorless     |

- |                                                 |                                                                                    |
|-------------------------------------------------|------------------------------------------------------------------------------------|
| c) Odor                                         | characteristic odour                                                               |
| d) Melting point/freezing point                 | Melting point: -14,5 °C at 1.013,25 hPa - Regulation (EC) No. 440/2008, Annex, A.1 |
| e) Initial boiling point and boiling range      | 199,5 °C at 1.013 hPa - OECD Test Guideline 103                                    |
| f) Flammability (solid, gas)                    | No data available                                                                  |
| g) Upper/lower flammability or explosive limits | Upper explosion limit: 20 %(V)<br>Lower explosion limit: 8,6 %(V)                  |
| h) Flash point                                  | 77 °C - Pensky-Martens closed cup                                                  |
| i) Autoignition temperature                     | 537 - 547 °C<br>at 1.019 hPa                                                       |
| j) Decomposition temperature                    | No data available                                                                  |
| k) pH                                           | No data available                                                                  |
| l) Viscosity                                    | Viscosity, kinematic: No data available<br>Viscosity, dynamic: 1,94 mPa.s at 23 °C |
| m) Water solubility                             | 2,1 g/l at 20 °C - soluble                                                         |
| n) Partition coefficient: n-octanol/water       | log Pow: 2,1 - Bioaccumulation is not expected.                                    |
| o) Vapor pressure                               | 0,51 hPa at 25 °C                                                                  |
| p) Density                                      | 1,088 g/cm <sup>3</sup>                                                            |
| Relative density                                | 1,08 at 20 °C - OECD Test Guideline 109                                            |
| q) Relative vapor density                       | 4,7 - (Air = 1.0)                                                                  |
| r) Particle characteristics                     | No data available                                                                  |
|                                                 |                                                                                    |
| s) Explosive properties                         | Not classified as explosive.                                                       |
| t) Oxidizing properties                         | none                                                                               |

## 9.2 Other safety information

|                        |                   |
|------------------------|-------------------|
| Relative vapor density | 4,7 - (Air = 1.0) |
|------------------------|-------------------|

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## SECTION 10: Stability and reactivity

### 10.1 Reactivity

Forms explosive mixtures with air on intense heating.  
A range from approx. 15 Kelvin below the flash point is to be rated as critical.

### 10.2 Chemical stability

The product is chemically stable under standard ambient conditions (room temperature) .

### 10.3 Possibility of hazardous reactions

Violent reactions possible with:

Strong oxidizing agents  
strong alkalis  
rubber  
various plastics

#### **10.4 Conditions to avoid**

Strong heating.

#### **10.5 Incompatible materials**

Strong oxidizing agents

#### **10.6 Hazardous decomposition products**

In the event of fire: see section 5

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### **SECTION 11: Toxicological information**

#### **11.1 Information on toxicological effects**

##### **Acute toxicity**

LD50 Oral - Rat - male - 1.625 mg/kg  
(OECD Test Guideline 401)  
Symptoms: Stomach/intestinal disorders, Nausea, Vomiting  
Acute toxicity estimate Oral - 1.625 mg/kg  
(ATE value derived from LD50/LC50 value)  
Inhalation: No data available  
Dermal: No data available

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

Skin - Rabbit  
Result: No skin irritation - 4 h  
(OECD Test Guideline 404)

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

Eyes - Rabbit  
Result: No eye irritation - 72 h  
(OECD Test Guideline 405)

##### **Respiratory or skin sensitization**

Local lymph node assay (LLNA) - Mouse  
Result: negative  
(OECD Test Guideline 429)

##### **Germ cell mutagenicity**

Test Type: Mutagenicity (mammal cell test): micronucleus.  
Test system: Human lymphocytes  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 487  
Result: negative  
Test Type: In vitro mammalian cell gene mutation test  
Test system: Chinese hamster lung cells  
Metabolic activation: with and without metabolic activation  
Method: OECD Test Guideline 476  
Result: negative

##### **Carcinogenicity**

No data available

##### **Reproductive toxicity**

Suspected of damaging the unborn child.

**Specific target organ toxicity - single exposure**

No data available

**Specific target organ toxicity - repeated exposure**

No data available

**Aspiration hazard**

No data available

## 11.2 Additional Information

### Endocrine disrupting properties

**Product:**

Assessment

The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher.

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

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Systemic effects:

Headache

Dizziness

Other dangerous properties can not be excluded.

Handle in accordance with good industrial hygiene and safety practice.

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## SECTION 12: Ecological information

### 12.1 Toxicity

Toxicity to fish                      semi-static test LC50 - Danio rerio (zebra fish) - 23 mg/l - 96 h  
(Regulation (EC) No. 440/2008, Annex, C.1)

Toxicity to algae                      static test ErC50 - Desmodesmus subspicatus (green algae) - 111,9  
mg/l - 72 h  
(Directive 67/548/EEC, Annex V, C.3.)

Toxicity to bacteria

### 12.2 Persistence and degradability

Biodegradability                      aerobic - Exposure time 29 d  
Result: 62 % - Readily biodegradable.  
(Regulation (EC) No. 440/2008, Annex, C.4-C)  
Remarks: The 10 day time window criterion is not fulfilled.

### 12.3 Bioaccumulative potential

No data available

No data available

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.

**Product:**

|            |                                                                                                                                                                                                                                                               |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Assessment | : The substance/mixture does not contain components considered to have endocrine disrupting properties according to REACH Article 57(f) or Commission Delegated regulation (EU) 2017/2100 or Commission Regulation (EU) 2018/605 at levels of 0.1% or higher. |
|------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|

Discharge into the environment must be avoided.

## No data available

ADR/RID: -

TMDG: -

IATA: -

ADR/RID: Not dangerous goods

IMDG: Not dangerous goods

IATA: Not dangerous goods

### Try next lesson: class(2)

ADR/RID: -

IMDG: -

IATA: -

ADR/RID: -

IMDG: -

IATA: -

ADR/RID: no

IMDG Marine pollutant: no

IATA: no

No data available

Further information : No data available

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

This material safety data sheet complies with the requirements of Regulation (EC) No. 1907/2006.

#### **Other regulations**

Observe work restrictions regarding maternity protection in accordance to Dir 92/85/EEC or stricter national regulations where applicable.

Take note of Dir 94/33/EC on the protection of young people at work.

#### **15.2 Chemical Safety Assessment**

For this product a chemical safety assessment was not carried out

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### **SECTION 16: Other information**

#### **Full text of H-Statements**

|       |                                         |
|-------|-----------------------------------------|
| H302  | Harmful if swallowed.                   |
| H361d | Suspected of damaging the unborn child. |

#### **Relevant changes since previous version**

2. Hazards identification  
9. Physical and chemical properties

CHEMIKART

## Full text of other abbreviations

ADN - European Agreement concerning the International Carriage of Dangerous Goods by Inland Waterways; ADR - Agreement concerning the International Carriage of Dangerous Goods by Road; AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; ELx - Loading rate associated with x% response; EmS - Emergency Schedule; ENCS - Existing and New Chemical Substances (Japan); ErCx - Concentration associated with x% growth rate response; GHS - Globally Harmonized System; GLP - Good Laboratory Practice; IARC - International Agency for Research on Cancer; IATA - International Air Transport Association; IBC - International Code for the Construction and Equipment of Ships carrying Dangerous Chemicals in Bulk; IC50 - Half maximal inhibitory concentration; ICAO - International Civil Aviation Organization; IECSC - Inventory of Existing Chemical Substances in China; IMDG - International Maritime Dangerous Goods; IMO - International Maritime Organization; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardization; KECI - Korea Existing Chemicals Inventory; LC50 - Lethal Concentration to 50 % of a test population; LD50 - Lethal Dose to 50% of a test population (Median Lethal Dose); MARPOL - International Convention for the Prevention of Pollution from Ships; n.o.s. - Not Otherwise Specified; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NZIoC - New Zealand Inventory of Chemicals; OECD - Organization for Economic Co-operation and Development; OPPTS - Office of Chemical Safety and Pollution Prevention; PBT - Persistent, Bioaccumulative and Toxic substance; PICCS - Philippines Inventory of Chemicals and Chemical Substances; (Q)SAR - (Quantitative) Structure Activity Relationship; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RID - Regulations concerning the International Carriage of Dangerous Goods by Rail; SADT - Self-Accelerating Decomposition Temperature; SDS - Safety Data Sheet; TCSI - Taiwan Chemical Substance Inventory; TECI - Thailand Existing Chemicals Inventory; TSCA - Toxic Substances Control Act (United States); UN - United Nations; UNRTDG - United Nations Recommendations on the Transport of Dangerous Goods; vPvB - Very Persistent and Very Bioaccumulative

## Further information

The information is believed to be correct but is not exhaustive and will be used solely as a guideline, which is based on current knowledge of the chemical substance or mixture and is applicable to appropriate safety precautions for the product. It does not represent any guarantee of the properties of the product. Sigma-Aldrich Corporation and its Affiliates shall not be held liable for any damage resulting from handling or from contact with the above product. See [www.sigma-aldrich.com](http://www.sigma-aldrich.com) and/or the reverse side of invoice or packing slip for additional terms and conditions of sale.

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