

SECTION 1. IDENTIFICATION

1.1 Product identifiers

Product name : Guaiacol, United States Pharmacopeia (USP)
Reference Standard

Product Number : 1300004
Brand : US Pharmacopeia
Index-No. : 604-031-00-6
CAS-No. : 90-05-1

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

Identified uses : Laboratory chemicals, Synthesis of substances

Restrictions on use : The product is being supplied under the TSCA R&D Exemption (40 CFR Section 720.36). It is the recipient's responsibility to comply with the requirements of the R&D exemption. The product may not be used for a non-exempt commercial purpose under TSCA unless appropriate consent is granted in writing by MilliporeSigma.

1.3 Details of the supplier of the safety data sheet

Company : Sigma-Aldrich Inc.
SPRUCE ST 3050
63103 St. Louis

Telephone : (314) 771-5765
Telefax: (800) 325-5052

1.4 Emergency telephone number

Emergency Phone # : 800 424 9300 (CHEMTREC) 24/7
+1 703 527 3887 (CHEMTREC) 24/7



SECTION 2. HAZARDS IDENTIFICATION

GHS classification in accordance with the OSHA Hazard Communication Standard (29 CFR 1910.1200)

Hazards for the product as supplied

Acute toxicity (Oral)	: Category 4
Skin irritation	: Category 2
Eye irritation	: Category 2A
Short-term (acute) aquatic hazard	: Category 3

Other hazards

None known.

GHS label elements

Hazard pictograms :



Signal word : Warning

Hazard statements : H302 Harmful if swallowed.
H315 Causes skin irritation.
H319 Causes serious eye irritation.
H402 Harmful to aquatic life.

Precautionary statements : **Prevention:**
P264 Wash skin thoroughly after handling.
P270 Do not eat, drink or smoke when using this product.
P273 Avoid release to the environment.
P280 Wear protective gloves/ eye protection/ face protection.
Response:
P301 + P312 + P330 IF SWALLOWED: Call a POISON CENTER/ doctor if you feel unwell. Rinse mouth.
P302 + P352 IF ON SKIN: Wash with plenty of soap and water.
P305 + P351 + P338 IF IN EYES: Rinse cautiously with water for several minutes. Remove contact lenses, if present and easy to do. Continue rinsing.
P332 + P313 If skin irritation occurs: Get medical advice/ attention.
P337 + P313 If eye irritation persists: Get medical



advice/ attention.
P362 Take off contaminated clothing and wash before reuse.

Disposal:

P501 Dispose of contents/ container to an approved waste disposal plant.

SECTION 3. COMPOSITION/INFORMATION ON INGREDIENTS

Substance / Mixture : Substance

CAS-No. : 90-05-1

Components

Chemical name	CAS No./Unique ID	Concentration (% w/w)	Trade secret
guaiacol	90-05-1*	>= 90 - <= 100	-

* Indicates that the identifier is a CAS No.

SECTION 4. FIRST AID MEASURES

General advice : Show this safety data sheet to the doctor in attendance.

If inhaled : After inhalation: fresh air.

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

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.

Most important symptoms and effects, both acute and delayed : The most important known symptoms and effects are described in the labelling (see section 2 GHS label elements) and/or in section 11

Protection of first-aiders : For personal protection see section 8.

Notes to physician : No data available



SECTION 5. FIREFIGHTING MEASURES

Unsuitable extinguishing media	: For this substance/mixture no limitations of extinguishing agents are given.
Hazardous combustion products	: Carbon oxides
Specific extinguishing methods	: No data available
Further information	: Prevent fire extinguishing water from contaminating surface water or the ground water system.
Special protective equipment for fire-fighters	: Stay in danger area only with self-contained breathing apparatus. Prevent skin contact by keeping a safe distance or by wearing suitable protective clothing.

SECTION 6. ACCIDENTAL RELEASE MEASURES

Personal precautions, protective equipment and emergency procedures	: Advice for non-emergency personnel: Avoid inhalation of dusts. Avoid substance contact. Ensure adequate ventilation. Evacuate the danger area, observe emergency procedures, consult an expert. Advice for emergency responders: Wear appropriate personal protective equipment, as indicated in Section 8.
Environmental precautions	: Do not let product enter drains.
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 dry. Dispose of properly. Clean up affected area. Avoid generation of dusts.

SECTION 7. HANDLING AND STORAGE

For precautions see section 2 GHS label elements



Further information on storage conditions : Tightly closed.
Dry.

Storage class : 11, Combustible Solids

Recommended storage temperature : 36 - 46 °F / 2 - 8 °C

SECTION 8. EXPOSURE CONTROLS/PERSONAL PROTECTION

Ingredients with workplace control parameters

Contains no substances with occupational exposure limit values.

Engineering measures : No data available

Personal protective equipment

Respiratory protection : required when dusts are generated.

Our recommendations on filtering respiratory protection are based on the following standards: DIN EN 143, DIN 14387 and other accompanying standards relating to the used respiratory protection system.

Recommended Filter type: : Filter type P2

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.

Hand protection

Remarks : required

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

Skin and body protection : protective clothing

Hygiene measures : Immediately change contaminated clothing. Apply preventive skin protection. Wash hands and face after working with substance.



SECTION 9. PHYSICAL AND CHEMICAL PROPERTIES

Appearance	: crystalline
Colour	: colourless
Odour	: strong, unpleasant
Odour Threshold	: No data available
pH	: No data available
Melting point/ range	: 81 - 84 °F / 27 - 29 °C
Boiling point/boiling range	: 401 °F / 205 °C (1013 hPa)
Flash point	: No data available
Evaporation rate	: No data available
Flammability (solid, gas)	: No data available
Flammability (liquids)	: No data available
Burning rate	: No data available
Self-ignition	: 707 °F / 375 °C 1,014 hPa
Upper explosion limit / Upper flammability limit	: No data available
Lower explosion limit / Lower flammability limit	: No data available
Vapour pressure	: 0.11 mmHg (77 °F / 25 °C)
Relative vapour density	: No data available
Relative density	: No data available
Density	: 1.129 g/cm ³
Solubility(ies) Water solubility	: 23.3 g/l completely soluble (77 °F / 25 °C)

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Partition coefficient: n-octanol/water	: log Pow: 1.36 - 1.57 Method: OECD Test Guideline 117
Autoignition temperature	: No data available
Decomposition temperature	: No data available
Viscosity, dynamic	: No data available
Viscosity, kinematic	: No data available
Flow time	: No data available
Explosive properties	: Not classified as explosive.
Oxidizing properties	: none
Molecular weight	: 124.14 g/mol
Particle characteristics Particle size	: No data available

SECTION 10. STABILITY AND REACTIVITY

Reactivity	: No data available
Chemical stability	: The product is chemically stable under standard ambient conditions (room temperature) .
Possibility of hazardous reactions	: No data available
Conditions to avoid	: Light. Air no information available
Incompatible materials	: Strong oxidizing agents Strong bases
Hazardous decomposition products	: For Hazardous combustion products in the event of fire: see section 5



SECTION 11. TOXICOLOGICAL INFORMATION

11.1 Information on toxicological effects

Acute toxicity

LD50 Oral - Mouse - male and female - 621 mg/kg
(OECD Test Guideline 401)

Inhalation: No data available

LD50 Dermal - Rabbit - 4,600 mg/kg

Remarks: (ECHA)

No data available

Skin corrosion/irritation

Skin - Rabbit

Result: Skin irritation - 4 h

(OECD Test Guideline 404)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Serious eye damage/eye irritation

Eyes - Rabbit

Result: Causes serious eye irritation.

(OECD Test Guideline 405)

Remarks: (Regulation (EC) No 1272/2008, Annex VI)

Respiratory or skin sensitization

Sensitisation test: - Guinea pig

Result: negative

Remarks: (ECHA)

Germ cell mutagenicity

Test Type: Ames test

Test system: *S. typhimurium*

Metabolic activation: with and without metabolic activation

Method: OECD Test Guideline 471

Result: negative

Test Type: Chromosome aberration test in vitro

Test system: Other cell types

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 473

Result: positive

Test Type: sister chromatid exchange assay

Test system: Other cell types

Metabolic activation: without metabolic activation

Method: OECD Test Guideline 479

Result: positive

Test Type: Micronucleus test

Species: Mouse

Cell type: Red blood cells (erythrocytes)

Application Route: Oral

Method: OECD Test Guideline 474

Result: negative



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.
- NTP: No component of this product present at levels greater than or equal to 0.1% is identified as a known or anticipated carcinogen by NTP.
- OSHA: No component of this product present at levels greater than or equal to 0.1% is on OSHA's list of regulated carcinogens.

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

11.2 Additional Information

Repeated dose toxicity - Rat - male - Oral - 4 Weeks - No observed adverse effect level - < 1,500 mg/kg - Lowest observed adverse effect level - 1,500 mg/kg
Remarks: (ECHA)

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

SECTION 12. ECOLOGICAL INFORMATION

Ecotoxicity

Components:

guaiacol:

Toxicity to daphnia and other aquatic invertebrates : EC50 (Daphnia magna (Water flea)): 25.9 mg/l
Exposure time: 48 h
Remarks: (ECOTOX Database)

Toxicity to algae/aquatic plants : ErC50 (Pseudokirchneriella subcapitata): > 100 mg/l
Exposure time: 72 h
Test Type: static test
Analytical monitoring: yes
Method: OECD Test Guideline 201
GLP: yes



Persistence and degradability

Components:

guaiacol:

Biodegradability : aerobic
Concentration: 100 mg/l
Result: Readily biodegradable.
Biodegradation: 90 %
Exposure time: 28 d
Method: OECD Test Guideline 301C

ThOD : 2,060 mg/g
Remarks: (Lit.)

Bioaccumulative potential

Components:

guaiacol:

Partition coefficient: n-octanol/water : log Pow: 1.36 - 1.57 (86 °F / 30 °C)
Method: OECD Test Guideline 117
Remarks: Bioaccumulation is not expected.

Mobility in soil

No data available

Other adverse effects

No data available

Endocrine disrupting properties

No data available

SECTION 13. DISPOSAL CONSIDERATIONS

Disposal methods

Waste from residues : Waste material must be disposed of in accordance with the national and local regulations. Leave chemicals in original containers. No mixing with other waste. Handle uncleaned containers like the product itself.

SECTION 14. TRANSPORT INFORMATION

International Regulations

IATA-DGR

Not regulated as a dangerous good

IMDG-Code

Not regulated as a dangerous good



Transport in bulk according to IMO instruments

Not applicable for product as supplied.

National Regulations

49 CFR

Not regulated as a dangerous good

Poison Inhalation Hazard : No

Special precautions for user

Remarks : Not classified as dangerous in the meaning of transport regulations.

SECTION 15. REGULATORY INFORMATION

CERCLA Reportable Quantity

This material does not contain any components with a CERCLA RQ.

SARA 304 Extremely Hazardous Substances Reportable Quantity

This material does not contain any components with a section 304 EHS RQ.

SARA 302 Extremely Hazardous Substances Threshold Planning Quantity

Components	CAS-No.	Component TPQ (lbs)
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SARA 311/312 Hazards : Acute Health Hazard

SARA 313 : 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.

US State Regulations

Massachusetts Right To Know

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

Pennsylvania Right To Know

guaiacol 90-05-1

Pennsylvania Right To Know

guaiacol 90-05-1

New Jersey Right To Know

guaiacol 90-05-1

California Prop. 65

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

The components of this product are reported in the following inventories:



US TSCA : All substances listed as active on the TSCA inventory

TSCA list

No substances are subject to a Significant New Use Rule.

No substances are subject to TSCA 12(b) export notification requirements.

SECTION 16. OTHER INFORMATION

Full text of other abbreviations

AIIC - Australian Inventory of Industrial Chemicals; ASTM - American Society for the Testing of Materials; bw - Body weight; CERCLA - Comprehensive Environmental Response, Compensation, and Liability Act; CMR - Carcinogen, Mutagen or Reproductive Toxicant; DIN - Standard of the German Institute for Standardisation; DOT - Department of Transportation; DSL - Domestic Substances List (Canada); ECx - Concentration associated with x% response; EHS - Extremely Hazardous Substance; 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; ERG - Emergency Response Guide; GHS - Globally Harmonised System; GLP - Good Laboratory Practice; HMIS - Hazardous Materials Identification System; 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 Organisation; ISHL - Industrial Safety and Health Law (Japan); ISO - International Organisation for Standardisation; 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; MSHA - Mine Safety and Health Administration; n.o.s. - Not Otherwise Specified; NFPA - National Fire Protection Association; NO(A)EC - No Observed (Adverse) Effect Concentration; NO(A)EL - No Observed (Adverse) Effect Level; NOELR - No Observable Effect Loading Rate; NTP - National Toxicology Program; NZIoC - New Zealand Inventory of Chemicals; OECD - Organisation 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; RCRA - Resource Conservation and Recovery Act; REACH - Regulation (EC) No 1907/2006 of the European Parliament and of the Council concerning the Registration, Evaluation, Authorisation and Restriction of Chemicals; RQ - Reportable Quantity; SADT - Self-Accelerating Decomposition Temperature; SARA - Superfund Amendments and Reauthorization Act; 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

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



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