



Formula: C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>

MW: 164.2

CAS: 97-53-0

MDL: MFCD00008654

TNP: TNP00389

SYNTHETIC CLOVE OIL; PHENOL, 4-ALLYL-2-METHOXY; 1,3,4-Eugenol;  
1-Allyl-4-hydroxy-3-methoxybenzene; 1-Hydroxy-2-methoxy-4-allylbenzene;  
1-Hydroxy-2-methoxy-4-prop-2-enylbenzene; 2-Hydroxy-5-allylanisole;  
2-Methoxy-1-hydroxy-4-allylbenzene



LogP: 3.55

LogS: -4.33

Acceptors: 2

Donors: 1

Rotation Bonds: 4

Chiral Centers: 0

N+O: 2

LIPINSKY: 4

Oil: LIQUID

Info: Eugenol 99%

IUPAC: 2-methoxy-4-prop-2-enylphenol

Smiles: c1(c(ccc(c1)CC=C)O)OC

Specification: Antioxidant; Biochemistry Eugenol Chemical Properties:

mp -12--10 C(lit.) bp 254 C(lit.) density 1.067 g/mL at 25 C(lit.) refractive index n<sub>20</sub>/D 1.541(lit.) FEMA 2467 Fp >230 F storage temp. 0-6C Water Solubility slightly soluble Merck 14,3898 BRN 1366759 Stability:Stable. Combustible. Incompatible with strong oxidizing agents. CAS DataBase Reference97-53-0(CAS DataBase Reference) NIST Chemistry ReferenceEugenol(97-53-0) EPA Substance Registry SystemPhenol, 2-methoxy-4-(2-propenyl)-(97-53-0) Safety Information Hazard Codes Xn Risk Statements 22-36/37/38-42/43-38-40 Safety Statements 26-36-24/25-23 WGK Germany 1 RTECS SJ4375000 F 10-23 HS Code 29095090 Hazardous Substances Data97-53-0(Hazardous Substances Data) Eugenol English Eugenol Usage And Synthesis Chemical Properties:

colourless to faintly yellow liquid with a strong odour of cloves General DescriptionClear colorless pale yellow or amber-colored liquid. Odor of cloves. Spicy pungent taste. Air & Water ReactionsDarkens and thickens on exposure to air. Also darkens with age. Eugenol may decompose on exposure to light. Insoluble in water. Reactivity ProfileEugenol is incompatible with strong oxidizers. This includes ferric chloride and potassium permanganate. Eugenol reacts with strong alkalis. Eugenol is incompatible with iron and zinc. Fire HazardEugenol is combustible. Eugenol Preparation ProductsVanillin-->ISOEUGENOL-->Clove oil-->EUGENOL ACETATE-->Methyl eugenol Raw materialsPotassium carbonate-->CARBON DIOXIDE-->Sodium acetate trihydrate-->Allyl chloride-->Linalool-->Guaiacol-->Allyl bromide-->Eucalyptus Citriodora Oil-->Clove oil-->Basil oil-->LAUREL OIL FROM LAURUS NOBILIS-->White camphor oil-->Allyl ether-->Cassia Aurantium P.E Catechins 8% HPLC-->CINNAMON LEAVES OIL-->OCIMENE-->Violet Leaf Absolute

Merck 13 Reference: Monograph Number: 0003931

Title: Eugenol

CAS Registry Number: 97-53-0

CAS Name: 2-Methoxy-4-(2-propenyl)phenol

Additional Names: 4-allyl-2-methoxyphenol; allylguaiacol; eugenic acid; caryophyllic acid

Molecular Formula: C<sub>10</sub>H<sub>12</sub>O<sub>2</sub>

Molecular Weight: 164.20.

Percent Composition: C 73.15%, H 7.37%, O 19.49%

Literature References: Obtained from many natural sources: Beilstein vol. 6, 961. Prepn: Claisen, Ann. 418, 113 (1919); from oil of cloves: Waterman, Priester, Rec. Trav. Chim. 48, 1272 (1929). Toxicity study: E. C. Hagan et al., Toxicol. Appl. Pharmacol. 7, 18 (1965).

Properties: Colorless or pale yellow liquid, bp 255. Darkens and thickens on exposure to air. Odor of cloves; spicy, pungent taste. mp -9.2 to -9.1. d420 1.0664. nD20 1.5410. Practically insol in water. Misc with alcohol, chloroform, ether, oils. One ml dissolves in 2 ml 70% alcohol; sol in glacial acetic acid, in aq fixed alkali hydroxide solns. Ferric chloride, potassium permanganate. LD50 in rats, mice (mg/kg): 2680, 3000 orally (Hagan).

Melting point: mp -9.2 to -9.1

Boiling point: bp 255

Index of refraction: nD20 1.5410

Density: d420 1.0664

Toxicity data: LD50 in rats, mice (mg/kg): 2680, 3000 orally (Hagan)

Derivative Type: Benzoate

Additional Names: O-Benzoyl Eugenol

Molecular Formula: C17H16O3

Molecular Weight: 268.31.

Percent Composition: C 76.10%, H 6.01%, O 17.89%

Properties: Crystals, mp 69-70. bp 360. Freely sol in benzene, chloroform, ether, hot alcohol. Practically insol in water.

Melting point: mp 69-70

Boiling point: bp 360

Use: In perfumery instead of oil of cloves; manuf vanillin. As insect attractant.

Therap-Cat: Analgesic (dental).