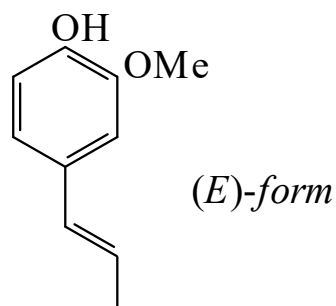




>>Entry Name: 2-Methoxy-4-(1-propenyl)phenol, 9CI

ENTRY UNDER REVIEW

Synonym(s): 4-Hydroxy-3-methoxy-1-propenylbenzene. 5-(1-Propenyl)guaiacol. **Isoeugenol**



CAS Registry Number: 97-54-1

Related CAS Registry Numbers(s): 93-29-8 61114-23-6 92666-21-2 119060-97-8 128839-47-4

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Biological Source: Occurs in ylang-ylang and other essential oils

Use/Importance: Used in perfumery and flavour industries, together with acetate and Me ether

Solubility: BERDY SOL: Sol. MeOH, Et₂O; fairly sol. H₂O

Other Data: Normally isol. as a mixt. of *E*- and *Z*-forms

Hazard & Toxicity: Skin irritant. LD₅₀ (rat, orl) 1560 mg/kg. Fl. p. >74/>100°

Aldrich: W24680-8

Fluka: 58850

Rare Chemicals Library: S42926-0

>>Variant: (*E*)-form

CAS Registry Number: 5932-68-3

Molecular Formula: C₁₀H₁₂O₂

Molecular Weight: 164.204

Accurate Mass: 164.08373

Percentage Composition: C 73.15%; H 7.37%; O 19.49%

Physical Description: Cryst.

Melting Point: Mp 33°

Boiling Point: Bp₁₂ 140-141°

pKa Value: pK_a 9.88 (25°)

Refractive Index: n_D²⁰ 1.5790

Other Data: λ_{max} 260 nm (ε 15135) (EtOH)

>>Derivative: *O*-β-D-Glucopyranoside

CAS Registry Number: 120442-72-0

Molecular Formula: C₁₆H₂₂O₇

Molecular Weight: 326.346

Accurate Mass: 326.136555

Percentage Composition: C 58.89%; H 6.79%; O 34.32%

Biological Source: Constit. of the petals of *Lilium cordatum*

Physical Description: Needles

Melting Point: Mp 170-174°

Optical Rotation: [α]_D²⁵ -39.4 (c, 1 in Py)

>>Derivative: Formyl

Synonym(s): Isoeugenyl formate. FEMA 2474