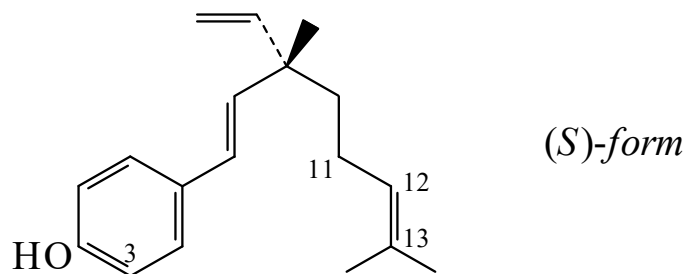




>>Entry Name: Bakuchiol

Synonym(s): 4-(3-Ethenyl-3,7-dimethyl-1,6-octadienyl)phenol, 9Cl. 1-(4-Hydroxyphenyl)-3,7-dimethyl-3-vinyl-1,6-octadiene. **Drupanol**‡



Related CAS Registry Numbers(s): 43010-46-4

Molecular Formula: C₁₈H₂₄O

Molecular Weight: 256.387

Accurate Mass: 256.182715

Percentage Composition: C 84.32%; H 9.43%; O 6.24%

Calculated Log P Data: Log P 6.13 (calc)

>>Variant: (S)-form

CAS Registry Number: 10309-37-2

Molecular Formula: C₁₈H₂₄O

Molecular Weight: 256.387

Accurate Mass: 256.182715

Percentage Composition: C 84.32%; H 9.43%; O 6.24%

Biological Source: Constit. of *Psoralea corylifolia*

Use/Importance: Antibacterial agent. Cytotoxic

Physical Description: Oil

Boiling Point: Bp_{0.7} 145-147°

Optical Rotation: [α]_D³⁰ +37.2

Solubility: BERDY SOL: Sol. bases, hexane, MeOH; poorly sol. H₂O

UV: [neutral] λ_{max} 261 (ε 16200) (MeOH) (Berdy) [neutral] λ_{max} 260 (ε 18400) (EtOH) (Berdy) [base] λ_{max} 285 (ε 20800) (EtOH-NaOH) (Berdy)

Other Data: Pharmacol. active isomer

Hazard & Toxicity: LD₅₀ (mus, orl) 2560 mg/kg. LD₅₀ (mus, ipr) 94 mg/kg ; BERDY HAZD : LD₅₀ (mus, ivn) 31 mg/kg , LD₅₀ (mus, ipr) 94 mg/kg , LD₅₀ (mus, orl) 2560 mg/kg

>>Derivative: Me ether

CAS Registry Number: 10309-44-1

Molecular Formula: C₁₉H₂₆O

Molecular Weight: 270.414

Percentage Composition: C 84.39%; H 9.69%; O 5.92%

Physical Description: Oil

Boiling Point: Bp_{0.13} 123-124°

>>Derivative: 12,13-Epoxyde

Synonym(s): 12,13-Epoxy-12,13-dihydrobakuchiol

Molecular Formula: C₁₈H₂₄O₂

Molecular Weight: 272.386

Accurate Mass: 272.17763

Percentage Composition: C 79.37%; H 8.88%; O 11.75%

Biological Source: Constit. of *Psoralea glandulosa*

Physical Description: Oil