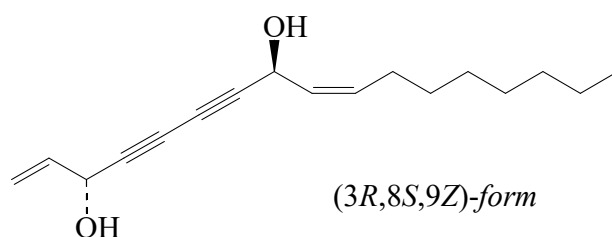




>>Entry Name: 1,9-Heptadecadiene-4,6-diyne-3,8-diol, 9C1
ENTRY UNDER REVIEW



CAS Registry Number: 30779-95-4

Molecular Formula: C₁₇H₂₄O₂
Molecular Weight: 260.375
Accurate Mass: 260.17763
Percentage Composition: C 78.42%; H 9.29%; O 12.29%
Calculated Log P Data: Log P 2.49 (calc)

>>Variant: (3R,8S,9Z)-form
Synonym(s): Falcarindiol

CAS Registry Number: 55297-87-5

Molecular Formula: C₁₇H₂₄O₂
Molecular Weight: 260.375
Accurate Mass: 260.17763
Percentage Composition: C 78.42%; H 9.29%; O 12.29%
Biological Source: Constit. of roots of several plants including the common carrot *Daucus carota* and *Angelica acutiloba*. Constit. of Chinese crude drug Toki
Biological Use/Importance: Has antifungal, antibiotic and analgesic activity. Antinociceptive agent
Physical Description: Pale yellow oil
Optical Rotation: [α]_D +204.8 (c, 1 in CHCl₃)
Solubility: BERDY SOL: Sol. MeOH, Et₂O
Calculated Log P Data: Log P 2.49 (calc)
UV: [neutral] λ_{max} 231 (); 244 (); 256 () (MeOH) (Berdy) [neutral] λ_{max} 233 (ε 1000); 245 (ε 1000); 259 (ε 800) (EtOH) (Berdy) [neutral] λ_{max} 232 (ε 400); 244 (ε 400); 258 (ε 200) (Et₂O) (Berdy)
Other Data: Pharmacol. active isomer

>>Derivative: 3-Ac

CAS Registry Number: 111264-34-7

Molecular Formula: C₁₉H₂₆O₃
Molecular Weight: 302.413
Accurate Mass: 302.188195
Percentage Composition: C 75.46%; H 8.67%; O 15.87%
Biological Source: Constit. of carrots

>>Derivative: 8-Ac

CAS Registry Number: 55249-27-9

Molecular Formula: C₁₉H₂₆O₃
Molecular Weight: 302.413
Accurate Mass: 302.188195
Percentage Composition: C 75.46%; H 8.67%; O 15.87%
Biological Source: Constit. of *Centella* spp. and *Polemannia montana*
UV: [neutral] λ_{max} 240 (ε 2238); 255 (ε 1943); 271 (ε 1940); 286 (ε 1660) (MeOH) (Berdy)

>>Derivative: 3-Ketone

Synonym(s): 8-Hydroxy-1,9-heptadecadien-4,6-diyn-3-one. **Falcarinolone**

CAS Registry Number: 18089-23-1

Molecular Formula: C₁₇H₂₂O₂
Molecular Weight: 258.36
Accurate Mass: 258.16198
Percentage Composition: C 79.03%; H 8.58%; O 12.39%
Biological Source: Isol. from *Carum carvi*, *Ligusticum mucronatum*, *Aegopodium*, *Angelica* spp. and *Daucus carota*
Physical Description: Unstable pale yellow oil
Optical Rotation: [α]