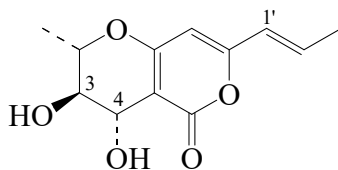




>>Entry Name: Radicinol



CAS Registry Number: 65647-66-7

Molecular Formula: C₁₂H₁₄O₅

Molecular Weight: 238.24

Accurate Mass: 238.084125

Percentage Composition: C 60.50%; H 5.92%; O 33.58%

Biological Source: Metab. of *Cochliobolus lunata*

Physical Description: Oil

Optical Rotation: [α]_D³¹ -175 (c, 1 in CHCl₃)

Solubility: BERDY SOL: Sol. MeOH, EtOAc

UV: [neutral] $\lambda_{\max}$ 226 (ϵ 39300); 262 (ϵ 3100); 271 (ϵ 3200); 318 (ϵ 10800) (EtOH) (Derep) [neutral] $\lambda_{\max}$ 224 (ϵ 28180); 260 (ϵ 3236); 271 (ϵ 3630); 315 (ϵ 8912) (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 226 (ϵ 39300); 262 (ϵ 3100); 271 (ϵ 3200); 318 (ϵ 10800) (EtOH) (Berdy)

>>Derivative: 4-Ketone

Synonym(s): Radicinin. Stemphylone

CAS Registry Number: 10088-95-6

Molecular Formula: C₁₂H₁₂O₅

Molecular Weight: 236.224

Accurate Mass: 236.068475

Percentage Composition: C 61.02%; H 5.12%; O 33.86%

Biological Source: Metab. of *Stemphylium radicinum*, *Alternaria chrysanthemi* and *Curvularia lunata*

Use/Importance: Active against gram-positive bacteria and fungi. Phytotoxin

Physical Description: Needles (EtOH)

Melting Point: Mp 238-240°

Optical Rotation: [α]_D²⁰ -236 (c, 0.1 in CHCl₃)

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

UV: [neutral] $\lambda_{\max}$ 271 (ϵ 7300); 280 (sh) (ϵ 5200); 340 (ϵ 21000) (EtOH) (Derep) [neutral] $\lambda_{\max}$ 215 (); 226 (); 348 () (MeOH) (Berdy) [neutral] $\lambda_{\max}$ 221 (ϵ 20600); 269 (ϵ 5250); 313 (ϵ 21300); 343 (ϵ 21500) (EtOH) (Berdy)

Rare Chemicals Library: S44847-8

Sigma: R3876

>>Derivative: 4-Ketone, Ac

Molecular Formula: C₁₄H₁₄O₆

Molecular Weight: 278.261

Accurate Mass: 278.07904

Percentage Composition: C 60.43%; H 5.07%; O 34.50%

Physical Description: Cryst.

Melting Point: Mp 197°

Optical Rotation: [α]_D²⁷ -267 (c, 0.7 in Py)

>>Derivative: 3-Deoxy, 4-ketone

Synonym(s): Deoxyradicinin

Molecular Formula: C₁₂H₁₂O₄

Molecular Weight: 220.224

Accurate Mass: 220.07356

Percentage Composition: C 65.45%; H 5.49%; O 29.06%

Biological Source: Phytoalexin from *Alternaria helianthi*

Physical Description: Cryst. (Me₂CO)

Melting Point: Mp 183-185°

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; poorly sol. C₆H₆, H₂O, hexane

UV: [neutral] $\lambda_{\max}$ 222 (ϵ 16200); 269 (ϵ 5250); 343 (ϵ 17700) (EtOH) (Berdy)