



>>Entry Name: 2,8,10-Heptadecatriene-4,6-diyne-1,14-diol

CAS Registry Number: 20311-78-8

H3CCH2CH2CH(OH)CH2CH2CH=CHCH=CHC#CC#CC=CHCH2OH

Molecular Formula: C₁₇H₂₂O₂

Molecular Weight: 258.36

Accurate Mass: 258.16198

Percentage Composition: C 79.03%; H 8.58%; O 12.39%

>>Variant: (2*E*,8*E*,10*E*,14*ξ*)-form

Synonym(s): Enanthotoxin. Oenanthotoxin

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 roots of *Oenanthe crocata*

Physical Description: Cryst. (C₆H₆ or MeOH)

Melting Point: Mp 87°

Optical Rotation: [α]_D¹⁵+30.5 (c, 2 in MeOH)

Hazard & Toxicity: Poisonous

>>Derivative: 1-Ac

CAS Registry Number: 20311-73-3

Molecular Formula: C₁₉H₂₄O₃

Molecular Weight: 300.397

Accurate Mass: 300.172545

Percentage Composition: C 75.97%; H 8.05%; O 15.98%

Biological Source: Isol. from *Oenanthe crocata*

Physical Description: Oil

>>Derivative: Di-Ac

Synonym(s): Centaur Z

Molecular Formula: C₂₁H₂₆O₄

Molecular Weight: 342.434

Accurate Mass: 342.18311

Percentage Composition: C 73.66%; H 7.65%; O 18.69%

Biological Source: Isol. from roots of *Centaurea montana*

Physical Description: Needles (pentane)

Melting Point: Mp 33°

Other Data: Probable structure

>>Variant: (2*Z*,8*E*,10*E*,14*ξ*)-form

Synonym(s): Bupleurotoxin

CAS Registry Number: 111128-27-9

Molecular Formula: C₁₇H₂₂O₂

Molecular Weight: 258.36

Accurate Mass: 258.16198

Percentage Composition: C 79.03%; H 8.58%; O 12.39%

Biological Source: Constit. of *Bupleurum longiradiatum*

Use/Importance: Toxin

Physical Description: Cryst. (MeOH)

Melting Point: Mp 54°

Optical Rotation: [α]_D¹⁸+20 (c, 0.02 in MeOH)