



>>Derivative: 7,8-Didehydro, 12-Ac, 3-*O*- β -D-xylopyranoside
Synonym(s): **Cimicifugoside**

CAS Registry Number: 66176-93-0

Molecular Formula: C₃₇H₅₄O₁₁
Molecular Weight: 674.827
Accurate Mass: 674.366615
Percentage Composition: C 65.85%; H 8.07%; O 26.08%
Biological Source: Constit. of *Cimicifuga simplex*
Physical Description: Cryst. (EtOH)
Melting Point: Mp 237-238°

>>Derivative: 7,8-Didehydro, 12-Ac, 3-*O*-(2-*O*-malonyl- β -D-xylopyranoside)
Synonym(s): **2'-*O*-Malonycimicifugoside**

CAS Registry Number: 245513-55-7

Molecular Formula: C₄₀H₅₆O₁₄
Molecular Weight: 760.874
Accurate Mass: 760.36701
Percentage Composition: C 63.14%; H 7.42%; O 29.44%
Biological Source: Constit. of *Cimicifuga simplex*
Physical Description: Powder
Optical Rotation: [α]_D -55.9 (c, 0.88 in MeOH)

>>Derivative: 26-Deoxy, 12-Ac
Synonym(s): **Deoxyacetylacteol**

Molecular Formula: C₃₂H₄₈O₆
Molecular Weight: 528.728
Accurate Mass: 528.34509
Percentage Composition: C 72.69%; H 9.15%; O 18.16%
Biological Source: Constit. of *Cimicifuga foetida*
Physical Description: Needles (EtOAc/hexane)
Melting Point: Mp 290-295°
Optical Rotation: [α]_D -80.4 (c, 0.16 in CHCl₃)