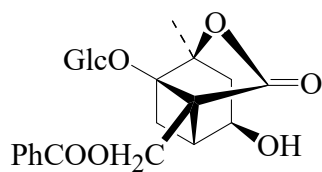




>>Entry Name: Albiflorin

Synonym(s): 9-[(Benzoyloxy)methyl]-1-(β-D-glucopyranosyloxy)-4-hydroxy-6-methyl-7-oxatricyclo[4.3.0.0^{3,9}]nonan-8-one, 9Cl



Absolute
Configuration

CAS Registry Number: 39011-90-0

Molecular Formula: C₂₃H₂₈O₁₁

Molecular Weight: 480.468

Accurate Mass: 480.163165

Percentage Composition: C 57.50%; H 5.87%; O 36.63%

Biological Source: Constit. of the oriental drug Shaoyao from *Paeonia albiflora* root

Biological Use/Importance: Anticonvulsant

Physical Description: Hygroscopic powder

Optical Rotation: [α]_D²² -19.9 (c, 0.95 in EtOH)

Calculated Log P Data: Log P -2.09 (uncertain value) (calc)

UV: [neutral] λ_{max} 231 (ε 11200); 267 (sh) (ε 1410); 274 (ε 1450); 281 (ε 1200) (EtOH) (Derep)

>>Derivative: 6'-O-Benzoyl

Synonym(s): Paeonivayin

CAS Registry Number: 184103-78-4

Molecular Formula: C₃₀H₃₂O₁₂

Molecular Weight: 584.576

Accurate Mass: 584.18938

Percentage Composition: C 61.64%; H 5.52%; O 32.84%

Biological Source: Constit. of *Paeonia delavayi*

Physical Description: Cryst.

Melting Point: Mp 152.5-155.5°

References:

Kaneda, M. *et al.*, *Tetrahedron*, 1972, **28**, 4309, (struct, uv)

Yamasaki, K. *et al.*, *Tet. Lett.*, 1976, 3965, (cmr)

Vollmer, K.O. *et al.*, *Z. Naturforsch., C*, 1986, **41**, 115, (hplc, metab)

Sugaya, A. *et al.*, *J. Ethnopharmacol.*, 1991, **33**, 159, (pharmacol)

Ma, Y.B. *et al.*, *Chin. Chem. Lett.*, 1999, **10**, 771-774, (Paeonivayin)