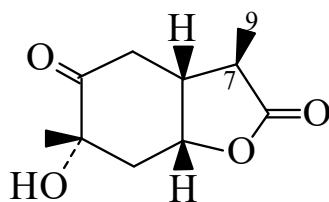




>>Entry Name: Paeonilactone A

Synonym(s): Tetrahydro-6-hydroxy-3,6-dimethyl-2,5(3*H*,4*H*)-benzofurandione, 9Cl



CAS Registry Number: 98751-79-2

Molecular Formula: C₁₀H₁₄O₄

Molecular Weight: 198.218

Accurate Mass: 198.08921

Percentage Composition: C 60.59%; H 7.12%; O 32.29%

Biological Source: Constit. of Paeony root

Physical Description: Needles (Et₂O/MeOH)

Melting Point: Mp 128-129°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -18.8$ (MeOH)

UV: [neutral] λ_{max} 215 (ϵ 6000) (MeOH) (Derep)

>>Derivative: 7,9-Didehydro

Synonym(s): Paeonilactone B

CAS Registry Number: 98751-78-1

Molecular Formula: C₁₀H₁₂O₄

Molecular Weight: 196.202

Accurate Mass: 196.07356

Percentage Composition: C 61.22%; H 6.16%; O 32.62%

Biological Source: Constit. of Paeony root

Physical Description: Needles (EtOAc)

Melting Point: Mp 88-89°

Optical Rotation: $[\alpha]_{\text{D}}^{25} +23.2$ (MeOH)

UV: [neutral] λ_{max} 215 (ϵ 6000) (MeOH) (Derep)

>>Derivative: 9-(Benzoyloxy)

Synonym(s): Paeonilactone C

CAS Registry Number: 98751-77-0

Molecular Formula: C₁₇H₁₈O₆

Molecular Weight: 318.326

Accurate Mass: 318.11034

Percentage Composition: C 64.14%; H 5.70%; O 30.16%

Biological Source: Constit. of Paeony root

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 132-133°

Optical Rotation: $[\alpha]_{\text{D}}^{25} -31.6$ (MeOH)

UV: [neutral] λ_{max} 229 (ϵ 63100); 267 (sh) (ϵ); 272 (ϵ 5130); 279 (sh) (ϵ) (MeOH) (Derep)

References:

- Hayashi, T. *et al.*, *Tet. Lett.*, 1985, **26**, 3699
Kadota, S. *et al.*, *Chem. Pharm. Bull.*, 1989, **37**, 843, (*synth*)
Richardson, D.P. *et al.*, *Tet. Lett.*, 1990, **31**, 5973, (*synth*)
Hatakeyama, S. *et al.*, *Tet. Lett.*, 1992, **33**, 333; 1994, **35**, 7993; 1995, **36**, 267, (*synth*)
Rönn, M. *et al.*, *Acta Chem. Scand.*, 1998, **52**, 524-527, (*synth*)
Boffey, R.J. *et al.*, *Chem. Comm.*, 1998, 1875-1876, (*synth*)
Jonasson, C. *et al.*, *J.O.C.*, 2000, **65**, 2122-2126, (*synth*)
Boffey, R. J. *et al.*, *J.C.S. Perkin I*, 2001, 487-496, (*synth*)