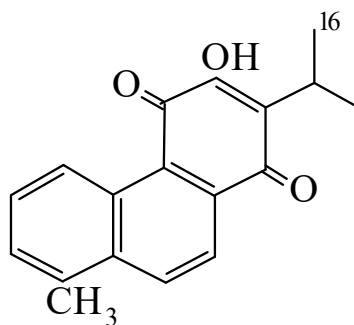




>>Entry Name: Danshenxinkun B

Synonym(s): 3-Hydroxy-2-isopropyl-8-methyl-1,4-phenanthraquinone



CAS Registry Number: 65907-76-8

Molecular Formula: C₁₈H₁₆O₃

Molecular Weight: 280.323

Accurate Mass: 280.109945

Percentage Composition: C 77.12%; H 5.75%; O 17.12%

Biological Source: Isol. from roots of *Salvia miltiorrhiza*

Physical Description: Orange-red needles

Melting Point: Mp 182°

>>Derivative: 16-Hydroxy

Synonym(s): Danshenxinkun A

CAS Registry Number: 65907-75-7

Molecular Formula: C₁₈H₁₆O₄

Molecular Weight: 296.322

Accurate Mass: 296.10486

Percentage Composition: C 72.96%; H 5.44%; O 21.60%

Biological Source: From roots of *Salvia miltiorrhiza*

Physical Description: Orange-yellow cryst.

Melting Point: Mp 200° (184-186°)

Optical Rotation: [α]_D²⁰ -33.5 (c, 0.09 in CHCl₃)

>>Derivative: 12-Deoxy

Synonym(s): 12-Deoxydanshenxinkun B

CAS Registry Number: 260397-57-7

Molecular Formula: C₁₈H₁₆O₂

Molecular Weight: 264.323

Accurate Mass: 264.11503

Percentage Composition: C 81.79%; H 6.10%; O 12.11%

Biological Source: Constit. of *Salvia glutinosa*

Physical Description: Red needles (CHCl₃/hexane)

Melting Point: Mp 187-197°

UV: [neutral] $\lambda_{\max}$ 289 (); 314 (sh) (); 423 () (CHCl₃) [neutral] $\lambda_{\max}$ 236 (); 288 (); 310 (sh) (); 421 () (MeOH)

References:

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Lee, A.R. *et al.*, *J. Nat. Prod.*, 1987, **50**, 157

Ikeshiro, Y. *et al.*, *Phytochemistry*, 1991, **30**, 2791, (*isol*, *pmr*, *cmr*)

Danheiser, R.L. *et al.*, *Tet. Lett.*, 1992, **33**, 1149, (*synth*)

Zhang, Z.-R. *et al.*, *Tet. Lett.*, 1994, **35**, 2153, (*synth*)

Nagy, G. *et al.*, *Phytochemistry*, 1999, **52**, 1105-1109, (*12-Deoxydanshenxinkun B*)