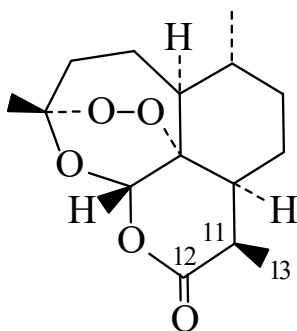




>>Entry Name: Artemisinin, INN

Synonym(s): Octahydro-3,6,9-trimethyl-3,12-epoxy-12*H*-pyrano[4,3-*j*]-1,2-benzodioxepin-10(3*H*)-one, 9Cl. Arteannuin. Qinghaosu. Qing Hau Sau. QHS



CAS Registry Number: 63968-64-9

Molecular Formula: C₁₅H₂₂O₅

Molecular Weight: 282.336

Accurate Mass: 282.146725

Percentage Composition: C 63.81%; H 7.85%; O 28.33%

General Statement: Eudesmane numbering shown

Biological Source: Constit. of *Artemisia annua* (Qinghaosu)

Use/Importance: Antimalarial agent. Shows advantages for use against drug-resistant malarial strains

Physical Description: Needles

Development Status: Extensively used in China, not yet approved for use in Western countries (1993)

Melting Point: Mp 156-157°

Optical Rotation: $[\alpha]_D^{17} +66.3$

Solubility: BERDY SOL: Sol. MeOH, C₆H₆; fairly sol. hexane; poorly sol. H₂O

Calculated Log P Data: Log P 1.68 (uncertain value) (calc)

UV: [neutral] $\lambda_{\max}$ 0 (end) (ϵ) (MeOH) (Derep) [neutral] $\lambda_{\max}$ (MeOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 5105 mg/kg. Exp. reprod. effects ; BERDY HAZD : LD₅₀ (mus, ims) 3840 mg/kg , LD₅₀ (mus, orl) 4228 mg/kg

Aldrich: 36159-3

Sigma: A5430

>>Derivative: 12β-Alcohol

Synonym(s): Dihydroqinghaosu. Dihydroartemisinin

CAS Registry Number: 71939-50-9

Molecular Formula: C₁₅H₂₄O₅

Molecular Weight: 284.352

Accurate Mass: 284.162375

Percentage Composition: C 63.36%; H 8.51%; O 28.13%

Biological Source: Isol. from qinghaosu

Use/Importance: Antimalarial agent

Physical Description: Cryst. (diisopropyl ether)

Melting Point: Mp 152-154°

Optical Rotation: $[\alpha]_D^{22} +129$ (c, 0.92 in CHCl₃)

Calculated Log P Data: Log P 1.78 (uncertain value) (calc)

>>Derivative: 12β-Alcohol, Me ether

Synonym(s): Artemether, INN

CAS Registry Number: 71963-77-4

Molecular Formula: C₁₆H₂₆O₅

Molecular Weight: 298.378

Accurate Mass: 298.178025

Percentage Composition: C 64.41%; H 8.78%; O 26.81%

Use/Importance: Antimalarial agent

Physical Description: Cryst. (hexane)

Melting Point: Mp 86-87°

Optical Rotation: $[\alpha]_D^{25} +163$ (c, 2.58 in CHCl₃)

Calculated Log P Data: Log P 2.24 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (mus, orl) 1000 mg/kg. LD₅₀ (mus, ims) 263 mg/kg. Exp. reprod. effects

>>Derivative: 12β-Alcohol, Et ether