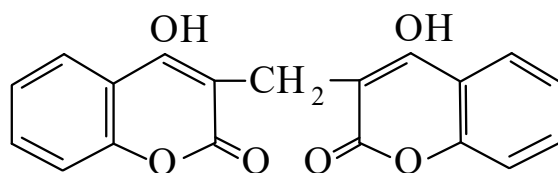




>>Entry Name: Dicoumarol, INN

Synonym(s): 3,3'-Methylenebis[4-hydroxy-2H-1-benzopyran-2-one], 9CI. 3,3'-Methylenebis-4-hydroxycoumarin, 8CI. Bishydroxycoumarin. Dicoumarin. Cumid. Dicumarol. Dufalone. Melitoxin. Many other names



CAS Registry Number: 66-76-2

Molecular Formula: C₁₉H₁₂O₆

Molecular Weight: 336.3

Accurate Mass: 336.06339

Percentage Composition: C 67.86%; H 3.60%; O 28.54%

Biological Source: Isol. from *Melilotus alba* and *Anthoxanthum* spp.

Use/Importance: Vitamin K antagonist. Orally active anticoagulant. Haemorrhagic agent causing ``sweet clover" disease in cattle. Antibacterial agent. Used as a 0.25-0.5% soln. in EtOH as turbidimetric acid-base indicator (pH range: 5.4-5.7)

Physical Description: Cryst. (cyclohexanone)

Melting Point: Mp 288-289°

Solubility: BERDY SOL: Sol. bases, Py; fairly sol. MeOH, Et₂O; poorly sol. H₂O, hexane

Calculated Log P Data: Log P 3.73 (calc)

UV: [neutral] λ_{max} 289 (ε 21200); 310 (ε 23460); 325 (ε 19320) (CHCl₃) (Berdy)

Hazard & Toxicity: Adverse effects reported (similar to Warfarin [CNP01-E](#)) when used therapeutically. Human and exp. reprod. effects. Exp. teratogen. LD₅₀ (rat, orl) 250 mg/kg ; BERDY HAZD : LD₅₀ (mus, scu) 200 - 300 mg/kg

Aldrich: 21893-6

Sigma: M1390

>>Derivative: Di-Ac

Molecular Formula: C₂₃H₁₆O₈

Molecular Weight: 420.375

Accurate Mass: 420.08452

Percentage Composition: C 65.72%; H 3.84%; O 30.45%

Physical Description: Cryst. (C₆H₆)

Melting Point: Mp 250-252 dec.°

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