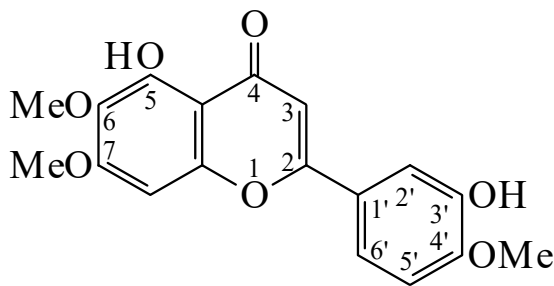




>>Entry Name: 3',5-Dihydroxy-4',6,7-trimethoxyflavone

Synonym(s): 5-Hydroxy-2-(3-hydroxy-4-methoxyphenyl)-6,7-dimethoxy-4*H*-1-benzopyran-4-one, 9Cl. Eupatorin‡



CAS Registry Number: 855-96-9

Type of Compound Code(s): VK5050 XA4050

Molecular Formula: C₁₈H₁₆O₇

Molecular Weight: 344.32

Accurate Mass: 344.089605

Percentage Composition: C 62.79%; H 4.68%; O 32.53%

Biological Source: Isol. from *Eupatorium semiserratum*, *Baccharis trimera*, *Centaurea aggregata*, *Sideritis altissimum* etc. and others in the Asteraceae and Labiatae

Use/Importance: Emetic

Physical Description: Yellow prisms (EtOH or dioxan aq.), needles (dioxan)

Melting Point: Mp 195-196°

Calculated Log P Data: Log P 0.82 (calc)

UV: [neutral] λ_{max} 243 (ε 17400); 254 (ε 19300); 274 (ε 19800); 342 (ε 27700) (EtOH) (Berdy)

Hazard & Toxicity: Cytotoxic

>>Derivative: Di-Ac

Molecular Formula: C₂₂H₂₀O₉

Molecular Weight: 428.395

Percentage Composition: C 61.68%; H 4.71%; O 33.61%

Physical Description: Needles

Melting Point: Mp 176-177°

References:

Kupchan, S.M. *et al.*, *J. Pharm. Sci.*, 1965, **54**, 929, (*isol, struct*)

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Adams, J.A. *et al.*, *Planta Med.*, 1977, **32**, 86, (*ms*)

Goudard, M. *et al.*, *Phytochemistry*, 1979, **18**, 186, (*ms*)

Iinuma, M. *et al.*, *Chem. Pharm. Bull.*, 1980, **28**, 708, (*cmr*)

Voirin, B. *et al.*, *Phytochemistry*, 1983, **22**, 2107, (*uv*)