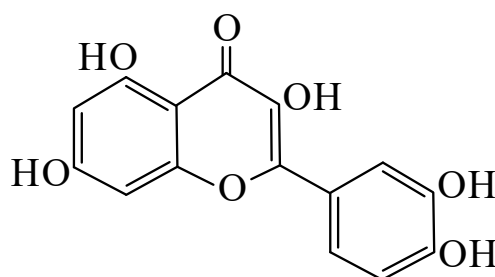




>>Entry Name: 3,3',4',5,7-Pentahydroxyflavone

ENTRY UNDER REVIEW

Synonym(s): 2-(3,4-Dihydroxyphenyl)-3,5,7-trihydroxy-4H-1-benzopyran-4-one, 9Cl. 3',4',5,7-Tetrahydroxyflavonol. **Quercetin**. Sophoretin. Meletin. Quercetol. Quertin. Ericin†



CAS Registry Number: 117-39-5

Related CAS Registry Numbers(s): 6151-25-3 6743-88-0 7215-44-3 7678-36-6 27214-55-7 90332-36-8 103666-99-5 116097-14-4 120537-33-9

Molecular Formula: C₁₅H₁₀O₇

Molecular Weight: 302.24

Accurate Mass: 302.042655

Percentage Composition: C 59.61%; H 3.33%; O 37.06%

Biological Source: Isol. from many plants, esp. fruits; *inter alia*, *Helichrysum*, *Euphorbia* and *Karwinskia* spp. Present in the Solanaceae, Rhamnaceae, Passifloraceae and many other families. For example detected in almost all studied Umbelliferae

Use/Importance: Used as soln. in EtOH for photometric detn. of Th ($\lambda_{\max}$ 422 nm, ϵ 33000), Al, Ga, In, Sc, Ta, Sn, Zr; fluorimetric detn. of Al. Antioxidant. Anticarcinogenic and antitumour promotor activities. Shows anti-HIV activity

Physical Description: Yellow cryst. + 2H₂O (EtOH aq.)

Melting Point: Mp 313-314 dec.°

Solubility: BERDY SOL: Sol. EtOH, Et₂O, bases; poorly sol. H₂O, hexane, CHCl₃

Calculated Log P Data: Log P -0.29 (calc)

UV: [neutral] $\lambda_{\max}$ 258 (ϵ 20900); 375 (ϵ 20900) (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, orl) 159 mg/kg. Exp. reprod. effects ; BERDY HAZD : LD₅₀ (mus, orl) 160 mg/kg

Rare Chemicals Library: S10272-5

>>Derivative: 3-O-Sulfate

CAS Registry Number: 97736-73-7

Molecular Formula: C₁₅H₁₀O₁₀S

Molecular Weight: 382.304

Accurate Mass: 381.99947

Percentage Composition: C 47.13%; H 2.64%; O 41.85%; S 8.39%

Biological Source: Isol. from *Ammi visnaga*, *Flaveria chloraefolia*, *Flaveria bidentis* and *Oenanthе crocata*

>>Derivative: 3'-O-Sulfate

CAS Registry Number: 62369-28-2

Molecular Formula: C₁₅H₁₀O₁₀S

Molecular Weight: 382.304

Accurate Mass: 381.99947

Percentage Composition: C 47.13%; H 2.64%; O 41.85%; S 8.39%

Biological Source: Isol. from *Hypericum elodes*

Physical Description: Yellow cryst.

>>Derivative: 3,3'-Di-O-sulfate

CAS Registry Number: 108909-05-3

Molecular Formula: C₁₅H₁₀O₁₃S₂

Molecular Weight: 462.368

Accurate Mass: 461.956285

Percentage Composition: C 38.97%; H 2.18%; O 44.98%; S 13.87%

Biological Source: Constit. of *Flaveria chloraefolia*