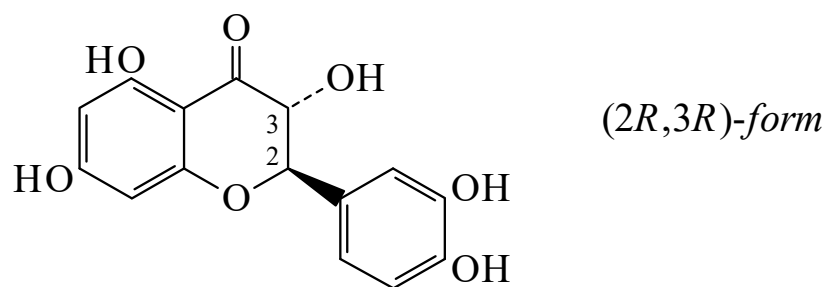




>>Entry Name: 3,3',4',5,7-Pentahydroxyflavanone

Synonym(s): 2-(3,4-Dihydroxyphenyl)-2,3-dihydro-3,5,7-trihydroxy-4H-1-benzopyran-4-one, 9Cl. 3',4',5,7-Tetrahydroxydihydroflavonol. Dihydroquercetin



CAS Registry Number: 98006-93-0

Related CAS Registry Numbers(s): 5117-01-1 17654-26-1 63393-40-8 64191-31-7 64191-33-9 82517-11-1 83680-48-2 117894-18-5

Molecular Formula: C₁₅H₁₂O₇

Molecular Weight: 304.256

Accurate Mass: 304.058305

Percentage Composition: C 59.22%; H 3.98%; O 36.81%

Calculated Log P Data: Log P 0.25 (uncertain value) (calc)

>>Variant: (2R,3R)-form

Synonym(s): (+)-trans-form. Taxifolin. Taxifoliol. Distylin

CAS Registry Number: 480-18-2

Molecular Formula: C₁₅H₁₂O₇

Molecular Weight: 304.256

Accurate Mass: 304.058305

Percentage Composition: C 59.22%; H 3.98%; O 36.81%

Biological Source: Appears to be the most widespread of the dihydroflavonols, present in the free state in the Leguminosae, Labiateae, Cactaceae, Erythroxylaceae, Illiciaceae, Polygonaceae, Salicaceae, Winteraceae, Ericaceae, Moraceae, Dilleniaceae, Eucryphiaceae, Coniferae, Hamamelidaceae, Myrtaceae, Balanophoraceae, Lauraceae, Sapotaceae, Anacardiaceae, Fagaceae, Rosaceae and Ericaceae

Biological Use/Importance: Antiinflammatory, antineoplastic and antifungal agent

Physical Description: Cryst. (EtOH or H₂O)

Melting Point: Mp 240-242° (221-222°)

Optical Rotation: $[\alpha]_D^{24} +44$ (c, 1.03 in 50% Me₂CO aq.)

Calculated Log P Data: Log P 0.25 (uncertain value) (calc)

Hazard & Toxicity: LD₅₀ (rat, ipr) 1200 mg/kg

Sigma: T4512

>>Derivative: 3-O-β-D-Apiofuranoside

CAS Registry Number: 124078-33-7

Molecular Formula: C₂₀H₂₀O₁₁

Molecular Weight: 436.371

Accurate Mass: 436.100565

Percentage Composition: C 55.05%; H 4.62%; O 40.33%

Biological Source: Constit. of the roots of *Rosa davurica*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_D -26$ (c, 1.1 in Me₂CO aq.)

>>Derivative: 3-O-α-L-Arabinofuranoside

Molecular Formula: C₂₀H₂₀O₁₁

Molecular Weight: 436.371

Accurate Mass: 436.100565

Percentage Composition: C 55.05%; H 4.62%; O 40.33%

Biological Source: Constit. of the roots of *Fragaria x ananassa*

Physical Description: Amorph. powder

Optical Rotation: $[\alpha]_D^{25} -32$ (c, 0.4 in MeOH)