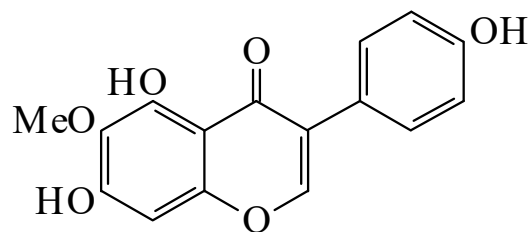




>>Entry Name: 4',5,7-Trihydroxy-6-methoxyisoflavone

Synonym(s): 5,7-Dihydroxy-3-(4-hydroxyphenyl)-6-methoxy-4H-1-benzopyran-4-one, 9Cl. Tectorigenin. K 251-T



CAS Registry Number: 548-77-6

Molecular Formula: C₁₆H₁₂O₆

Molecular Weight: 300.267

Accurate Mass: 300.06339

Percentage Composition: C 64.00%; H 4.03%; O 31.97%

Biological Source: Isol. from *Baptisia* spp., *Centrosema* spp., *Dalbergia* spp. and *Ononis spinosa* (all Leguminosae, Papilionoideae) and also *Iris germanica*

Biological Use/Importance: Antiinflammatory agent

Physical Description: Yellow plates (EtOH) or needles (C₆H₆/EtOH)

Melting Point: Mp 235-237° (227° dec.)

Solubility: BERDY SOL: Sol. EtOAc

Calculated Log P Data: Log P 0.63 (calc)

UV: [neutral] λ_{max} 268 (ε 30000) (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (mus, ipr) 3000 mg/kg

>>Derivative: 7-O-β-D-Glucopyranoside

Synonym(s): Tectoridin. Shekanin. Shekkanin

CAS Registry Number: 611-40-5

Molecular Formula: C₂₂H₂₂O₁₁

Molecular Weight: 462.409

Accurate Mass: 462.116215

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Source: Isol. from *Baptisia* spp., *Belamcanda chinensis*, *Dalbergia* spp., *Iris* spp. and *Pueraria montana*

Biological Use/Importance: Antiinflammatory agent

Physical Description: Needles

Melting Point: Mp 257 dec.°

Optical Rotation: [α]_D²⁰ -29.4 (Py)

Calculated Log P Data: Log P -2.43 (calc)

>>Derivative: 4'-O-β-D-Glucopyranoside

CAS Registry Number: 141894-63-5

Molecular Formula: C₂₂H₂₂O₁₁

Molecular Weight: 462.409

Accurate Mass: 462.116215

Percentage Composition: C 57.14%; H 4.80%; O 38.06%

Biological Source: Constit. of *Iris crocea*

Physical Description: Cream needles (MeOH)

Melting Point: Mp 187°

>>Derivative: 7-O-[β-D-Xylopyranosyl-(1→6)-β-D-glucopyranoside]

Molecular Formula: C₂₇H₃₀O₁₅

Molecular Weight: 594.525

Accurate Mass: 594.158475

Percentage Composition: C 54.55%; H 5.09%; O 40.37%

Biological Source: Constit. of the flowers of *Pueraria thunbergiana*

Physical Description: Pale yellow powder (MeOH)

Optical Rotation: [α]_D²⁵ -43.3 (c, 0.15 in DMSO)

UV: [neutral] λ_{max} 273 (); 336 () (MeOH)

Other Data: Mp >300°