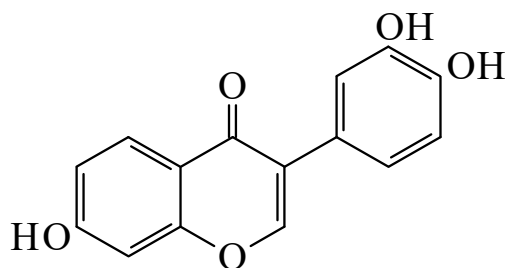




>>Entry Name: 3',4',7-Trihydroxyisoflavone

Synonym(s): 3-(3,4-Dihydroxyphenyl)-7-hydroxy-4H-1-benzopyran-4-one, 9Cl. 3'-Hydroxydaidzein



CAS Registry Number: 485-63-2

Molecular Formula: C₁₅H₁₀O₅

Molecular Weight: 270.241

Accurate Mass: 270.052825

Percentage Composition: C 66.67%; H 3.73%; O 29.60%

Biological Source: Isol. from heartwood of *Machaerium villosum*, *Machaerium mucronulatum* and *Streptomyces* sp. OH-1049

Use/Importance: Antioxidant

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 262-265° (252°). Mp 276-280°

Solubility: BERDY SOL: Sol. MeOH, HCl; poorly sol. H₂O

UV: [acid] λ_{max} (no shifts reported) (Derep) [base] λ_{max} 257 (ε); 335 (ε) (MeOH/NaOH) (Derep) [neutral] λ_{max} 248 (ε); 259 (ε); 292 (ε) (MeOH) (Derep) [acid] λ_{max} 259 (); 292 () (MeOH-HCl) (Berdy)

Other Data: All isolations of isoflavonoids from microorganisms are considered suspect

>>Derivative: 3'-Me ether

Synonym(s): 4',7-Dihydroxy-3'-methoxyisoflavone. 3'-Methoxydaidzein

CAS Registry Number: 21913-98-4

Molecular Formula: C₁₆H₁₂O₅

Molecular Weight: 284.268

Accurate Mass: 284.068475

Percentage Composition: C 67.60%; H 4.25%; O 28.14%

Biological Source: Isol. from *Cyclobium claussemi*, *Maackia amurensis* and *Machaerium villosum*

Physical Description: Plates (MeOH)

Melting Point: Mp 262°

>>Derivative: 3'-Me ether, 7-O-β-D-glucopyranoside

Synonym(s): 3'-Methoxydaidzin

Molecular Formula: C₂₂H₂₂O₁₀

Molecular Weight: 446.41

Accurate Mass: 446.1213

Percentage Composition: C 59.19%; H 4.97%; O 35.84%

Biological Source: Constit. of *Pueraria lobata*

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 226-228°

Optical Rotation: [α]_D -24.3 (c, 0.1 in DMSO)

UV: [neutral] λ_{max} 202 (log ε 4.5); 219 (log ε 4.46); 249 (sh) (log ε 4.31); 265 (log ε 4.4); 291 (sh) (log ε 4.18) (EtOH)

>>Derivative: 4'-Me ether

Synonym(s): 3',7-Dihydroxy-4'-methoxyisoflavone. Calycosin. 3-Hydroxyformononetin

CAS Registry Number: 20575-57-9

Molecular Formula: C₁₆H₁₂O₅

Molecular Weight: 284.268

Accurate Mass: 284.068475

Percentage Composition: C 67.60%; H 4.25%; O 28.14%

Biological Source: Isol. from *Baptisia*, *Bowdichia*, *Cadia*, *Cladrastis*, *Cyclobium*, *Dalbergia*, *Machaerium*, *Myroxylon*, *Pterocarpus*, *Sophora*, *Thermopsis* and *Trifolium* spp. (all Leguminosae subfamily Papilionoideae)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 245-247° (228-230°)