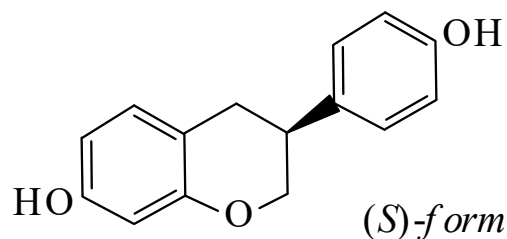




>>Entry Name: 4',7-Dihydroxyisoflavan

Synonym(s): 3,4-Dihydro-3-(4-hydroxyphenyl)-2H-benzopyran-7-ol. Equol



CAS Registry Number: 94105-90-5

Related CAS Registry Numbers(s): 89019-86-3

Molecular Formula: C₁₅H₁₄O₃

Molecular Weight: 242.274

Accurate Mass: 242.094295

Percentage Composition: C 74.36%; H 5.82%; O 19.81%

>>Variant: (S)-form

CAS Registry Number: 531-95-3

Molecular Formula: C₁₅H₁₄O₃

Molecular Weight: 242.274

Accurate Mass: 242.094295

Percentage Composition: C 74.36%; H 5.82%; O 19.81%

Biological Source: Isol. from heartwood of *Millettia pendula*. Metabolite found in human urine and urine of cows, goats and other animals

Physical Description: Cryst. (EtOH aq.)

Melting Point: Mp 189-190.5°

Optical Rotation: $[\alpha]_{\text{Hg}}$ -21.5

>>Derivative: Di-Ac

CAS Registry Number: 21140-91-0

Physical Description: Cryst. (MeOH)

Melting Point: Mp 122.5°

>>Derivative: 4'-Me ether

Synonym(s): 7-Hydroxy-4'-methoxyisoflavan. 4'-O-Methylequol

Molecular Formula: C₁₆H₁₆O₃

Molecular Weight: 256.301

Accurate Mass: 256.109945

Percentage Composition: C 74.98%; H 6.29%; O 18.73%

Biological Source: Found in sheeps' urine

>>Derivative: 7-Me ether

Synonym(s): 4'-Hydroxy-7-methoxyisoflavan

Molecular Formula: C₁₆H₁₆O₃

Molecular Weight: 256.301

Accurate Mass: 256.109945

Percentage Composition: C 74.98%; H 6.29%; O 18.73%

Biological Source: Constit. of bovine urine

Physical Description: Cryst. (CHCl₃/hexane)

Melting Point: Mp 150-151°

>>Derivative: Di-Me ether

Synonym(s): 4',7-Dimethoxyisoflavan

CAS Registry Number: 4366-35-2

Molecular Formula: C₁₇H₁₈O₃

Molecular Weight: 270.327

Accurate Mass: 270.125595

Percentage Composition: C 75.53%; H 6.71%; O 17.76%

Physical Description: Cryst. (MeOH)

Melting Point: Mp 89°

Optical Rotation: $[\alpha]$