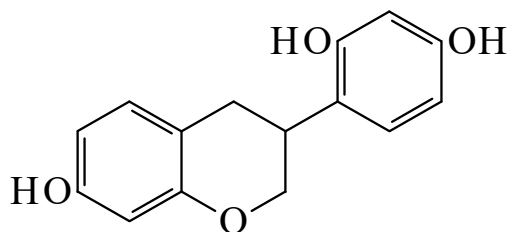




>>Entry Name: **2',4',7-Trihydroxyisoflavan**

Synonym(s): 4-(3,4-Dihydro-7-hydroxy-2*H*-1-benzopyran-4-yl)-1,3-benzenediol, 9CI. 3,4-Dihydro-3-(2,4-dihydroxyphenyl)-7-hydroxy-2*H*-1-benzopyran. **Demethylvestitol**



CAS Registry Number: 65332-45-8

Related CAS Registry Numbers(s): 64190-84-7 75556-92-2

Molecular Formula: C₁₅H₁₄O₄

Molecular Weight: 258.273

Accurate Mass: 258.08921

Percentage Composition: C 69.76%; H 5.46%; O 24.78%

Biological Source: Isol. from *Anthyllis vulneraria*, *Erythrina sandwicensis*, *Hosackia americana*, *Lablab niger*, *Lotus* spp., *Phaseolus vulgaris* and *Tetragonolobus* spp. as a phytoalexin

UV: [neutral] $\lambda_{\max}$ 209 (); 283 () (EtOH) (Berdy) [base] $\lambda_{\max}$ 219 (); 297 () (EtOH-NaOH) (Berdy)

>>Derivative: 2'-Me ether

Synonym(s): 4',7-Dihydroxy-2'-methoxyisoflavan. **Isovestitol**

CAS Registry Number: 63631-42-5

Molecular Formula: C₁₆H₁₆O₄

Molecular Weight: 272.3

Accurate Mass: 272.10486

Percentage Composition: C 70.58%; H 5.92%; O 23.50%

Biological Source: Phytoalexin of *Anthyllis vulneraria*, *Erythrina sandwicensis*, *Hosackia americana*, *Lablab niger*, *Tetragonolobus* spp. and *Trifolium* spp.

Physical Description: Needles

Melting Point: Mp 95-97°

UV: [neutral] $\lambda_{\max}$ 209 (); 282 () (EtOH) (Berdy) [base] $\lambda_{\max}$ 219 (); 243 (); 295 () (EtOH-NaOH) (Berdy)

>>Derivative: 4'-Me ether

>>Derivative: 7-Me ether

Synonym(s): 2',4'-Dihydroxy-7-methoxyisoflavan. **Neovestitol**

CAS Registry Number: 71772-21-9

Molecular Formula: C₁₆H₁₆O₄

Molecular Weight: 272.3

Accurate Mass: 272.10486

Percentage Composition: C 70.58%; H 5.92%; O 23.50%

Biological Source: Isol. from leaves of *Dalbergia sericea*

UV: [neutral] $\lambda_{\max}$ 212 (); 284 (); 289 () (EtOH) (Berdy) [base] $\lambda_{\max}$ 215 (); 291 () (EtOH-NaOH) (Berdy)

>>Derivative: 2',4'-Di-Me ether

Synonym(s): 7-Hydroxy-2',4'-dimethoxyisoflavan. **Sativan**. Sativin. 2'-*O*-Methylvestitol

CAS Registry Number: 41743-86-6

Molecular Formula: C₁₇H₁₈O₄

Molecular Weight: 286.327

Accurate Mass: 286.12051

Percentage Composition: C 71.31%; H 6.34%; O 22.35%

Biological Source: Isol. from *Derris amazonica*, and phytoalexin of *Lotus* spp., *Medicago* spp., *Trifolium* spp. and *Trigonella* spp.

Physical Description: Cryst.

Melting Point: Mp 128-129° (125-127°)

Optical Rotation: $[\alpha]_D^{22}$ -15

UV: [neutral] $\lambda_{\max}$ 286 () (MeOH) (Berdy)

Other Data: Mp. refers to the (*S*)-enantiomer from *D. amazonica*