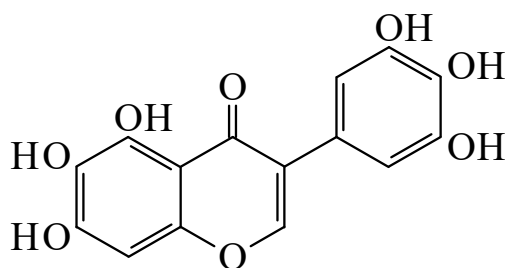




>>Entry Name: 3',4',5,5',6,7-Hexahydroxyisoflavone

Synonym(s): 5,6,7-Trihydroxy-3-(3,4,5-trihydroxyphenyl)-4*H*-1-benzopyran-4-one. Irigenol



CAS Registry Number: 4935-93-7

Molecular Formula: C<sub>15</sub>H<sub>10</sub>O<sub>8</sub>

Molecular Weight: 318.239

Accurate Mass: 318.03757

Percentage Composition: C 56.61%; H 3.17%; O 40.22%

Physical Description: Pale-yellow cryst. + 1H<sub>2</sub>O

Melting Point: Mp 330-330.5 dec.°

>>Derivative: 3',4',6-Tri-Me ether

Synonym(s): 3',5,7-Trihydroxy-4',5',6-trimethoxyisoflavone. **Irigenin**

CAS Registry Number: 548-76-5

Molecular Formula: C<sub>18</sub>H<sub>16</sub>O<sub>8</sub>

Molecular Weight: 360.32

Accurate Mass: 360.08452

Percentage Composition: C 60.00%; H 4.48%; O 35.52%

Biological Source: Constit. of several *Iris* spp. and of *Juniperus macropoda*

Use/Importance: Shows antifungal props.

Physical Description: Pale-yellow needles or plates (EtOH aq.)

Melting Point: Mp 185°

>>Derivative: 3',4',6-Tri-Me ether, 7-*O*-β-D-glucopyranoside

Synonym(s): **Iridin**

CAS Registry Number: 491-74-7

Molecular Formula: C<sub>24</sub>H<sub>26</sub>O<sub>13</sub>

Molecular Weight: 522.462

Accurate Mass: 522.137345

Percentage Composition: C 55.17%; H 5.02%; O 39.81%

Biological Source: From *Iris* spp., *Belamcanda chinensis* and *Juniperus macropoda*

Physical Description: Needles (MeOH aq.)

Melting Point: Mp 208°

>>Derivative: 3',4',6-Tri-Me ether, 5-*O*-[4-hydroxy-3-methoxybenzoyl-(→6)-β-D-glucopyranoside]

Synonym(s): **Shigansu A**

CAS Registry Number: 189282-16-4

Molecular Formula: C<sub>32</sub>H<sub>32</sub>O<sub>16</sub>

Molecular Weight: 672.595

Accurate Mass: 672.16904

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

Biological Source: Constit. of *Belamcanda chinensis*

Physical Description: Yellow cryst.

Melting Point: Mp 140-143°

Optical Rotation:  $[\alpha]_D^{14} -17.3$  (c, 0.2 in EtOH)

UV: [neutral]  $\lambda_{\max}$  265 (log  $\epsilon$  4.79) (no solvent reported)