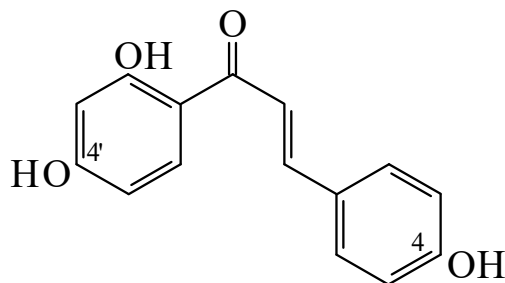




>>Entry Name: 2',4,4'-Trihydroxychalcone

Synonym(s): 1-(2,4-Dihydroxyphenyl)-3-(4-hydroxyphenyl)-2-propen-1-one. **Isoliquiritigenin**



CAS Registry Number: 961-29-5

Related CAS Registry Numbers(s): 2198-19-8 13745-20-5 23141-04-0 27233-96-1 30925-62-3 32274-67-2

Molecular Formula: C₁₅H₁₂O₄

Molecular Weight: 256.257

Accurate Mass: 256.07356

Percentage Composition: C 70.31%; H 4.72%; O 24.97%

Biological Source: Isol. from *Sophora tomentosa*, *Dalbergia* spp., *Onobrychis vicifolia*, *Medicago* spp., *Machaerium* spp., *Lespedeza cyrtobotrya*, *Dahlia tenuicaulis*, *Dahlia variabilis*, *Acacia* spp., *Platymiscium* spp., *Cyclolobium* and others. Widespread in the Leguminosae and Compositae

Use/Importance: Aldose reductase inhibitor. Shows antineoplastic and antiinflammatory activity

Physical Description: Pale yellow needles (EtOAc/petrol or EtOH aq.)

Melting Point: Mp 200-204° (198-200°)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃; poorly sol. H₂O, hexane

Calculated Log P Data: Log P 2.25 (calc)

UV: [neutral] λ_{max} 285 (); 328 (); 368 () (MeOH) (Berdy) [base] λ_{max} 428 () (MeOH-NAOH) (Berdy)

Sigma: I3766

>>Derivative: 4-O-β-D-Glucopyranoside

Synonym(s): **Isoliquiritin**. Isoliquiritoside

CAS Registry Number: 5041-81-6

Molecular Formula: C₂₁H₂₂O₉

Molecular Weight: 418.399

Accurate Mass: 418.126385

Percentage Composition: C 60.28%; H 5.30%; O 34.42%

Biological Source: Isol. from *Trifolium subterraneum*, *Glycyrrhiza* spp. and others

Use/Importance: Antiinflammatory agent

Melting Point: Mp 187-189°

Optical Rotation: [α]_D -60.8

Calculated Log P Data: Log P -0.57 (calc)

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

Synonym(s): **Neoisoliquiritin**

CAS Registry Number: 59122-93-9

Molecular Formula: C₂₁H₂₂O₉

Molecular Weight: 418.399

Accurate Mass: 418.126385

Percentage Composition: C 60.28%; H 5.30%; O 34.42%

Biological Source: Isol. from *Glycyrrhiza glabra*, *Cicer arietinum*, *Dahlia* spp., *Glycine max*, *Ulex europaeus* and others

Use/Importance: Antiinflammatory agent

Physical Description: Yellow needles (EtOH)

Melting Point: Mp 230-232°

Optical Rotation: [α]_D -61.5 (c, 0.5 in EtOH)

Calculated Log P Data: Log P -0.59 (calc)