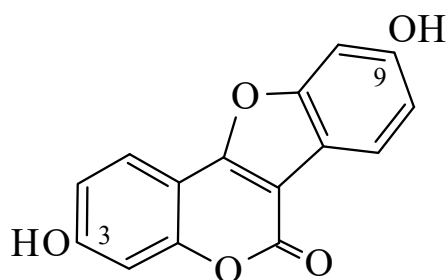




>>Entry Name: Coumestrol

ENTRY UNDER REVIEW

Synonym(s): 3,9-Dihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, 9Cl. 3,9-Dihydroxycoumestan. 7,12-Dihydroxycoumestan (obsol.). 3,9-Dihydroxy-6-oxopterocarpen (obsol.). 6',7-Dihydroxybenzofuro[3',2',3,4]coumarin (obsol.). Cumostrol



CAS Registry Number: 479-13-0

Molecular Formula: C₁₅H₈O₅

Molecular Weight: 268.225

Accurate Mass: 268.037175

Percentage Composition: C 67.17%; H 3.01%; O 29.82%

Biological Source: Isol. from *Medicago* spp., *Glycine max*, *Astragalus sinicus*, *Centrosema pubescens*, *Dolichos biflorus*, *Melilotus alba*, *Phaseolus* spp. *Pisum sativum*, *Psoralea corylifolia*, *Trifolium* spp., *Trigonella corniculata* and *Vigna unguiculata* (all Leguminosae, subfam. Papilionoideae), also from *Spinacea oleracea* (Chenopodiaceae) and *Brassica oleracea* (Cruciferae)

Use/Importance: Binds to estrogen receptor sites in human breast cancer cells (MCF-7) *in vitro*. Estrogenic agent

Melting Point: Mp 385°

Solubility: BERDY SOL: Sol. bases; fairly sol. MeOH, CHCl₃, Et₂O; poorly sol. H₂O, C₆H₆, CCl₄, acids

Calculated Log P Data: Log P 3.12 (calc)

UV: [neutral] λ_{max} 208 (); 243 (); 343 () (MeOH) (Berdy) [neutral] λ_{max} 243 (); 307 (); 343 () (EtOH) (Berdy) [base] λ_{max} 250 (); 280 (); 310 (); 385 () (NAOH) (Berdy)

Other Data: Subl. at 325°. Shows blue fluorescence

Hazard & Toxicity: Exp. reprod. and teratogenic effects

Fluka: 27885

>>Derivative: 3-*O*-β-D-Glucopyranoside

Synonym(s): Coumestrin

CAS Registry Number: 92631-72-6

Molecular Formula: C₂₁H₁₈O₁₀

Molecular Weight: 430.367

Accurate Mass: 430.09

Percentage Composition: C 58.61%; H 4.22%; O 37.18%

Biological Source: Constit. of *Glycine max*

Physical Description: Oil

>>Derivative: 3-Me ether

Synonym(s): 3-*O*-Methylcoumestrol

Molecular Formula: C₁₆H₁₀O₅

Molecular Weight: 282.252

Accurate Mass: 282.052825

Percentage Composition: C 68.09%; H 3.57%; O 28.34%

Biological Source: Isol. from alfalfa (*Medicago sativa*)

Physical Description: Cryst. (Me₂CO/MeOH)

Melting Point: Mp 331-332°

>>Derivative: 9-Me ether

Synonym(s): 9-*O*-Methylcoumestrol. 3-Hydroxy-9-methoxycoumestan

CAS Registry Number: 1690-62-6

Molecular Formula: C₁₆H₁₀O₅

Molecular Weight: 282.252

Accurate Mass: 282.052825

Percentage Composition: C 68.09%; H 3.57%; O 28.34%

Biological Source: Isol. from *Cicer arietinum*, *Dalbergia oliveri*, *Dalbergia stevensonii*, *Medicago* spp., *Myroxylon balsamum*, *Pisum sativum*, *Trifolium pratense*, *Trifolium repens* and *Sophora tomentosa*