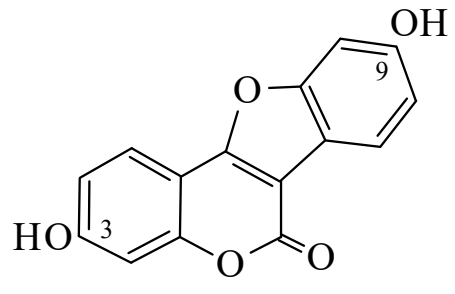
>>**Entry Name: Coumestrol**
ENTRY UNDER REVIEW
Synonym(s): 3,9-Dihydroxy-6*H*-benzofuro[3,2-*c*][1]benzopyran-6-one, 9Cl. 3,9-Dihydroxycoumestan. 7,12-Dihydroxycoumestan (obsol.). 3,9-Dihydroxy-6-oxopterocarpen (obsol.). 6',7-Dihydroxybenzofuro[3',2',3,4]coumarin (obsol.). Cumostrol



CAS Registry Number: 479-13-0

Molecular Formula: $C_{15}H_8O_5$
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, $CHCl_3$, Et_2O; poorly sol. H_2O, C_6H_6, CCl_4, 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: $C_{21}H_{18}O_{10}$
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: $C_{16}H_{10}O_5$
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. (Me_2CO/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: $C_{16}H_{10}O_5$
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*