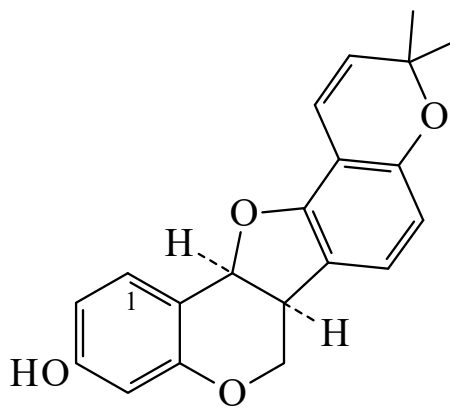




>>Entry Name: Phaseollin

Synonym(s): 6*b*,12*b*-Dihydro-3,3-dimethyl-3*H*,7*H*-furo[3,2-*c*:5,4-*f*]bis[1]benzopyran-10-ol, 9*Cl*. Phaseolin



Absolute
conf guration

CAS Registry Number: 13401-40-6

Molecular Formula: C₂₀H₁₈O₄

Molecular Weight: 322.36

Accurate Mass: 322.12051

Percentage Composition: C 74.52%; H 5.63%; O 19.85%

Biological Source: Isol. from *Phaseolus vulgaris*. Also found in *Erythrina abyssinica* and *Vigna unguiculata*

Use/Importance: Active against bacteria, fungi and yeasts. Phytoalexin

Melting Point: Mp 177-178°

Optical Rotation: [α]_D −145 (c, 0.17 in EtOH)

Solubility: BERDY SOL: Sol. MeOH, Et₂O, bases; fairly sol. H₂O

pKa Value: p*K*_a 9.13

Calculated Log P Data: Log P 3.96 (uncertain value) (calc)

UV: [neutral] λ_{max} 207 (ε 47900); 230 (ε 25100); 280 (ε 9330); 286 (ε 7940); 315 (ε 2190) (MeOH) (Derep) [neutral] λ_{max} 279 (ε 9120); 286 (ε 7940); 315 (ε 2190) (EtOH) (Berdy) [base] λ_{max} 281 (ε 11480); 292 (ε 10960); 377 (ε 2880) (EtOH-NaOH) (Berdy)

>>Derivative: 1-Methoxy

Synonym(s): 1-Methoxyphaseollin

CAS Registry Number: 157226-48-7

Molecular Formula: C₂₁H₂₀O₅

Molecular Weight: 352.386

Accurate Mass: 352.131075

Percentage Composition: C 71.58%; H 5.72%; O 22.70%

Biological Source: Constit. of the roots of *Glycyrrhiza glabra*

Physical Description: Yellowish oil

Optical Rotation: [α]_D²⁵ −16.7 (c, 0.91 in MeOH)

References:

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Kamat, V.S. *et al.*, *Heterocycles*, 1981, **15**, 1163, (*isol*)
Dewick, P.M. *et al.*, *Phytochemistry*, 1982, **21**, 1599, (*biosynth*)
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Mohamed, S.E.N. *et al.*, *J.C.S. Perkin I*, 1987, 431, (*synth*)
Kitagawa, I. *et al.*, *Chem. Pharm. Bull.*, 1994, **42**, 1056, (*1-Methoxyphaseollin*)