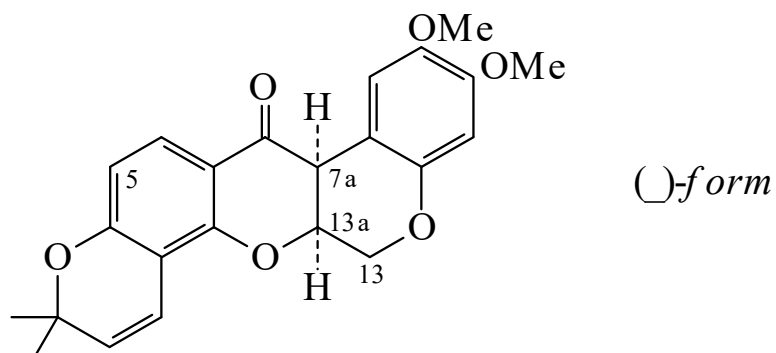




>>Entry Name: Deguelin

Synonym(s): 13,13a-Dihydro-9,10-dimethoxy-3,3-dimethyl-3*H*-bis[1]benzopyrano[3,4-*b*:6',5'-*e*]pyran-7(7*aH*)one, 9Cl. Isodeguelin



CAS Registry Number: 522-17-8

Molecular Formula: C₂₃H₂₂O₆

Molecular Weight: 394.423

Accurate Mass: 394.14164

Percentage Composition: C 70.04%; H 5.62%; O 24.34%

General Statement: CA numbering shown

>>Variant: (-)-form

Molecular Formula: C₂₃H₂₂O₆

Molecular Weight: 394.423

Accurate Mass: 394.14164

Percentage Composition: C 70.04%; H 5.62%; O 24.34%

Biological Source: Isol. from *Crotalaria burhia*, *Derris elliptica*, *Derris malaccensis*, *Lonchocarpus* spp., *Millettia ferruginea*, *Millettia pachycarpa*, *Mundulea sericea*, *Piscidia mollis* and *Tephrosia* spp. (all Leguminosae, Papilionoideae)

Physical Description: Cryst. (EtOH)

Melting Point: Mp 171°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -101$ (C₆H₆)

Other Data: Occurs as partial racemates

Hazard & Toxicity: Strong irritant, toxic by inhalation

>>Derivative: 7*a*,13*a*-Didehydro

Synonym(s): Dehydrodeguelin

CAS Registry Number: 3466-23-7

Molecular Formula: C₂₃H₂₀O₆

Molecular Weight: 392.407

Accurate Mass: 392.12599

Percentage Composition: C 70.40%; H 5.14%; O 24.46%

Biological Source: Isol. from *Amorpha fruticosa*, *Derris elliptica*, *Millettia dura*, *Tephrosia candida* and *Tephrosia vogelii*

Physical Description: Yellow cryst. or thick yellow prisms (CHCl₃/MeOH)

Melting Point: Mp 232-233° (217°)

>>Derivative: 13*R*-Hydroxy

Synonym(s): 13-Hydroxydeguelin

CAS Registry Number: 158784-67-9

Molecular Formula: C₂₃H₂₂O₇

Molecular Weight: 410.423

Accurate Mass: 410.136555

Percentage Composition: C 67.31%; H 5.40%; O 27.29%

Biological Source: Constit. of the bark of *Mundulea sericea*

Physical Description: Yellowish cryst. (MeOH)

Melting Point: Mp 179°

Optical Rotation: $[\alpha]_{\text{D}}^{20} -14$ (c, 0.13 in CHCl₃)