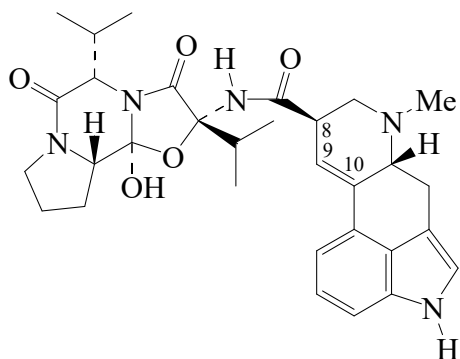




>>Entry Name: Ergocornine

Synonym(s): 12'-Hydroxy-2',5'-bis(1-methylethyl)ergotaman-3',6',18-trione, 9Cl



CAS Registry Number: 564-36-3

Related CAS Registry Numbers(s): 8006-25-5 8047-28-7

Molecular Formula: C₃₁H₃₉N₅O₅

Molecular Weight: 561.68

Accurate Mass: 561.29512

Percentage Composition: C 66.29%; H 7.00%; N 12.47%; O 14.24%

Biological Source: Alkaloid from ergot (*Claviceps purpurea*)

Use/Importance: Vasoconstrictor. Investigational tool for studying ovum implantation in mammals. Pharmacol. effects resemble those of Ergotamine [BCL03-C](#) but is more toxic and little used clinically

Melting Point: Mp 182-184 dec.°

Optical Rotation: $[\alpha]_D^{20}$ -175 (c, 1 in CHCl₃). $[\alpha]_D$ -110 (c, 1 in Py)

Solubility: BERDY SOL: Sol. Me₂CO, CHCl₃, EtOAc; fairly sol. EtOH; poorly sol. H₂O

Calculated Log P Data: Log P 5.07 (uncertain value) (calc)

UV: [neutral] $\lambda_{\max}$ 311 (ϵ 8130) (MeOH) (Berdy)

Other Data: Component of Ergotoxine

Hazard & Toxicity: Exp. reprod. effects ; BERDY HAZD : LD₅₀ (rbt, ivn) 1.17 mg/kg

>>Derivative: Me ether

Synonym(s): 12'-O-Methylergocornine

CAS Registry Number: 112767-18-7

Molecular Formula: C₃₂H₄₁N₅O₅

Molecular Weight: 575.706

Accurate Mass: 575.31077

Percentage Composition: C 66.76%; H 7.18%; N 12.16%; O 13.90%

Biological Source: Alkaloid from *Claviceps purpurea*

>>Derivative: 9,10 α -Dihydro

Synonym(s): Dihydroergocornine

CAS Registry Number: 25447-65-8

Extra CAS Registry Numbers(s): 5611-87-0

Molecular Formula: C₃₁H₄₁N₅O₅

Molecular Weight: 563.695

Accurate Mass: 563.31077

Percentage Composition: C 66.05%; H 7.33%; N 12.42%; O 14.19%

Melting Point: Mp 185-187 dec.°

Optical Rotation: $[\alpha]_D^{20}$ -48 (c, 0.5 in Py)

>>Derivative: 8-Epimer

Synonym(s): Ergocorninine

CAS Registry Number: 564-37-4

Molecular Formula: C₃₁H₃₉N₅O₅

Molecular Weight: 561.68

Accurate Mass: 561.29512

Percentage Composition: C 66.29%; H 7.00%; N 12.47%; O 14.24%

Biological Source: Alkaloid from ergot

Physical Description: Prisms (MeOH)

Melting Point: Mp 228 dec.°

Optical Rotation: $[\alpha]$ +500 (c, 1.0 in Py)