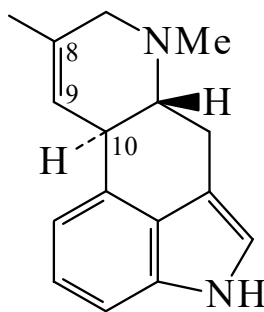




>>Entry Name: Agroclavine

Synonym(s): 8,9-Didehydro-6,8-dimethylergoline, 9CI



Absolute
configuration

Molecular Formula: C₁₆H₁₈N₂

Molecular Weight: 238.332

Accurate Mass: 238.146998

Percentage Composition: C 80.63%; H 7.61%; N 11.75%

>>Variant: (-)-form

CAS Registry Number: 548-42-5

Molecular Formula: C₁₆H₁₈N₂

Molecular Weight: 238.332

Accurate Mass: 238.146998

Percentage Composition: C 80.63%; H 7.61%; N 11.75%

Biological Source: Alkaloid from ergot and from several spp. in the genera *Argyreia*, *Rivea*, *Cuscuta*, *Ipomoea* (Convolvulaceae) and *Penicillium* spp.

Use/Importance: CNS excitator acting by stimulation of sympathetic centres

Melting Point: Mp 208-209 dec.°

Optical Rotation: [α]_D -151 (CHCl₃). [α]_D -182 (Py)

Solubility: BERDY SOL: Sol. MeOH, CHCl₃, Py; fairly sol. C₆H₆; poorly sol. H₂O

UV: [neutral] $\lambda_{\max}$ 225 (ϵ 29512); 284 (ϵ 7586); 293 (ϵ 6456) (MeOH) (Berdy)

Hazard & Toxicity: BERDY HAZD : LD₅₀ (mus, ipr) 25 mg/kg

>>Derivative: Dihydro

see Festuclavine, [GNZ79-X](#)

>>Derivative: 10-Epimer

Synonym(s): Agroclavine I

CAS Registry Number: 82597-81-7

Molecular Formula: C₁₆H₁₈N₂

Molecular Weight: 238.332

Accurate Mass: 238.146998

Percentage Composition: C 80.63%; H 7.61%; N 11.75%

Biological Source: Metab. of *Penicillium kapuscinskii* strain UCM F-2156D

UV: [neutral] $\lambda_{\max}$ 211 (sh) (ϵ 14600); 225 (ϵ 25500); 276 (sh) (ϵ); 282 (ϵ 5470); 292 (ϵ 4560) (MeOH) (Derep)

>>Derivative: 10-Epimer, 8 β ,9 β -epoxide

Synonym(s): Epoxyagroclavine I

CAS Registry Number: 82564-34-9

Molecular Formula: C₁₆H₁₈N₂O

Molecular Weight: 254.331

Accurate Mass: 254.141913

Percentage Composition: C 75.56%; H 7.13%; N 11.01%; O 6.29%

Biological Source: Metab. from *Penicillium kapuscinskii*

UV: [neutral] $\lambda_{\max}$ 211 (sh) (ϵ 14600); 225 (ϵ 25500); 276 (sh) (ϵ); 282 (ϵ 5470); 292 (ϵ 4560) (MeOH) (Derep)