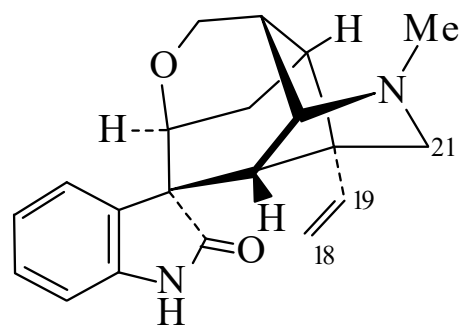




>>Entry Name: Gelsemine, 9CI



Relative
configuration

CAS Registry Number: 509-15-9

Molecular Formula: $C_{20}H_{22}N_2O_2$

Molecular Weight: 322.406

Accurate Mass: 322.168128

Percentage Composition: C 74.51%; H 6.88%; N 8.69%; O 9.93%

Biological Source: Alkaloid from *Gelsemium sempervirens*, *Gelsemium elegans* and *Mostuea stimulans* (Loganiaceae)

Use/Importance: Analgesic, CNS stimulant. Gelsemium Root has been used to treat trigeminal neuralgia and migraine. Also used in homoeopathic medicine

Melting Point: Mp 178°

Optical Rotation: $[\alpha]_D^{20} +17.8$ (c, 2.03 in $CHCl_3$)

Calculated Log P Data: Log P 0.48 (uncertain value) (calc)

Hazard & Toxicity: V. toxic. *G. spp.* have been freq. causes of human poisoning. LD₅₀ (mus, ipr) 49 mg/kg. CNS depressant, can cause respiratory arrest

Sigma: G2750

>>Derivative: Hydrochloride

Melting Point: Mp 333 dec.° (rapid heating)

pKa Value: pK_a 9.79 (13°)

>>Derivative: Hydrobromide

Physical Description: Prisms (EtOH aq.)

Melting Point: Mp 325 dec.°

>>Derivative: Picrate

Physical Description: Yellow plates (MeOH)

Melting Point: Mp 203°

>>Derivative: Methobromide

Physical Description: Needles (EtOH)

Melting Point: Mp 313-314°

>>Derivative: Methiodide

Melting Point: Mp 286-301 dec.° (variable)

Optical Rotation: $[\alpha]_D^{18} +6$ (c, 0.93 in H_2O)

>>Derivative: *N*-Methoxy

Synonym(s): Gelseverine. *N*-Methoxygelsemine. Alkaloid A‡

CAS Registry Number: 38990-03-3

Molecular Formula: $C_{21}H_{24}N_2O_3$

Molecular Weight: 352.432

Accurate Mass: 352.178693

Percentage Composition: C 71.57%; H 6.86%; N 7.95%; O 13.62%

Biological Source: Alkaloid from *Gelsemium sempervirens* and *Gelsemium elegans* (Loganiaceae)

Physical Description: Oil

Melting Point: Mp 245°

Optical Rotation: $[\alpha]_D -4.5$