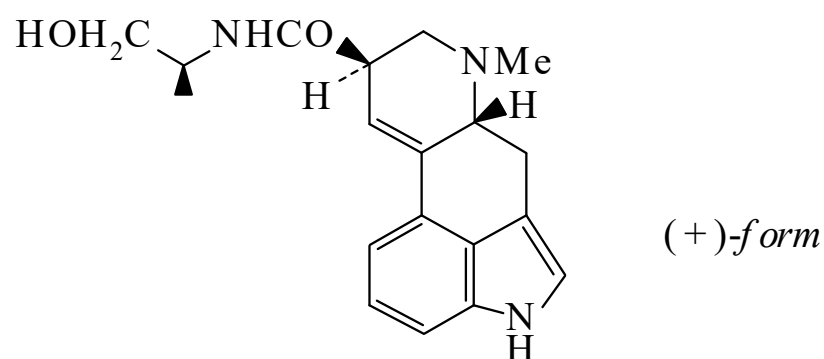




>>Entry Name: Ergometrine, BAN, INN

Synonym(s): 9,10-Didehydro-*N*-(2-hydroxy-1-methylethyl)-6-methylergoline-8-carboxamide, 9Cl. Ergonovine. Ergotrate. Ergobasine. Ergotocin. Ergostetrine



Related CAS Registry Numbers(s): 129-50-0

Molecular Formula: C<sub>19</sub>H<sub>23</sub>N<sub>3</sub>O<sub>2</sub>

Molecular Weight: 325.41

Accurate Mass: 325.179027

Percentage Composition: C 70.13%; H 7.12%; N 12.91%; O 9.83%

Use/Importance: 5HT receptor antagonist. Oxytocic agent used in childbirth. Shows little adrenolytic or CNS effect

Calculated Log P Data: Log P 1.03 (uncertain value) (calc)

>>Variant: (+)-form

CAS Registry Number: 60-79-7

Molecular Formula: C<sub>19</sub>H<sub>23</sub>N<sub>3</sub>O<sub>2</sub>

Molecular Weight: 325.41

Accurate Mass: 325.179027

Percentage Composition: C 70.13%; H 7.12%; N 12.91%; O 9.83%

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

Use/Importance: 5-Hydroxytryptamine antagonist

Physical Description: Plates (EtOAc), needles (Me<sub>2</sub>CO)

Melting Point: Mp 162-163 dec.°. Mp 212 dec.° (dimorph.)

Other Data: Pharmacol. active isomer

Hazard & Toxicity: Adverse systemic effects by intramuscular route. LD<sub>50</sub> (mus, ivn) 144 mg/kg

Sigma: E3129

>>Derivative: Hydrochloride

Melting Point: Mp 245-246 dec.°

Optical Rotation:  $[\alpha]_D^{25} +63$  (H<sub>2</sub>O)

>>Derivative: Picrate

Physical Description: Red prisms or hydrated yellow needles

Melting Point: Mp 188-189 dec.° (anhyd.). Mp 148 dec.° (hydrated)

>>Derivative: Maleate

Synonym(s): Ergonovine maleate, USAN. Ergometrine maleate, JAN. Cornocentin. Ermetrine. Syntometrine. Many other names

CAS Registry Number: 129-51-1

Use/Importance: Used in the prevention and treatment of postpartum haemorrhage

Melting Point: Mp 167 dec.°

Optical Rotation:  $[\alpha]_D^{25} +48$

Hazard & Toxicity: Adverse effects reported when used therapeutically. LD<sub>50</sub> (mus, ivn) 8.26 mg/kg

Sigma: E6500