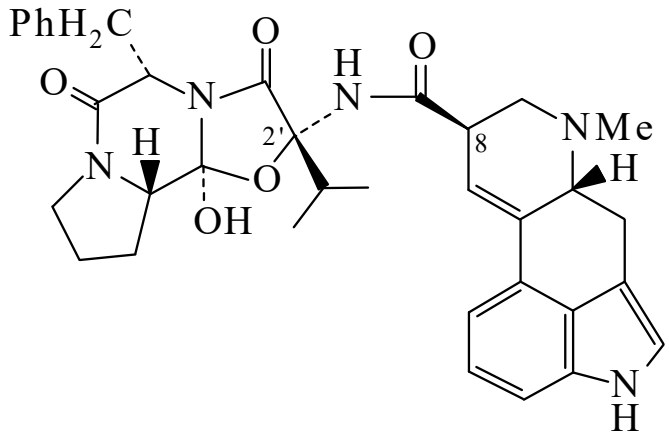
>>**Entry Name: Ergocristine**
Synonym(s): 12'-Hydroxy-2'-(1-methylethyl)-5'-(phenylmethyl)ergotaman-3',6',18-trione, 9CI



Absolute conf guration

CAS Registry Number: 511-08-0
Related CAS Registry Numbers(s): 8006-25-5 8067-24-1

Molecular Formula: $C_{35}H_{39}N_5O_5$
Molecular Weight: 609.724
Accurate Mass: 609.29512
Percentage Composition: C 68.95%; H 6.45%; N 11.49%; O 13.12%
Biological Source: Alkaloid from ergot (*Claviceps purpurea*)
Biological Use/Importance: Vasoconstrictor. Pharmacol. effects resemble those of Ergotamine BCL03-C but is more toxic, therefore little used clinically
Melting Point: Mp 165-170°
Optical Rotation: $[\alpha]_D^{20}$ –173 (c, 0.7 in $CHCl_3$). $[\alpha]_D$ –101 (c, 0.8 in Py)
Calculated Log P Data: Log P 5.56 (uncertain value) (calc)
Other Data: Component of Ergotoxine

Sigma: E6000

>>**Derivative:** 9,10-Dihydro
Synonym(s): Dihydroergocristine, BAN**.** Many other names

CAS Registry Number: 17479-19-5

Molecular Formula: $C_{35}H_{41}N_5O_5$
Molecular Weight: 611.739
Accurate Mass: 611.31077
Percentage Composition: C 68.72%; H 6.76%; N 11.45%; O 13.08%
Biological Use/Importance: Used in treatment of impaired mental function in the elderly. Peripheral and cerebral vasodilator
Calculated Log P Data: Log P 5.86 (uncertain value) (calc)
Other Data: Mainly used as a mix. with other dihydroergot alkaloids
Sigma: D6253

>>**Derivative:** 9,10-Dihydro; methanesulfonate
Synonym(s): Dihydroergocristine mesilate, BAN

CAS Registry Number: 24730-10-7

>>**Derivative:** 8-Epimer
Synonym(s): Ergocristinine

CAS Registry Number: 511-07-9

Molecular Formula: $C_{35}H_{39}N_5O_5$
Molecular Weight: 609.724
Accurate Mass: 609.29512
Percentage Composition: C 68.95%; H 6.45%; N 11.49%; O 13.12%
Biological Source: Alkaloid from ergot
Physical Description: Prisms (MeOH)
Melting Point: Mp 226-227 dec.° (214° dec.)
Optical Rotation: $[\alpha]_D^{20}$+370 (c, 0.4 in $CHCl_3$). $[\alpha]_D^{20}$+471 (c, 0.35 in Py)
Sigma: E6250