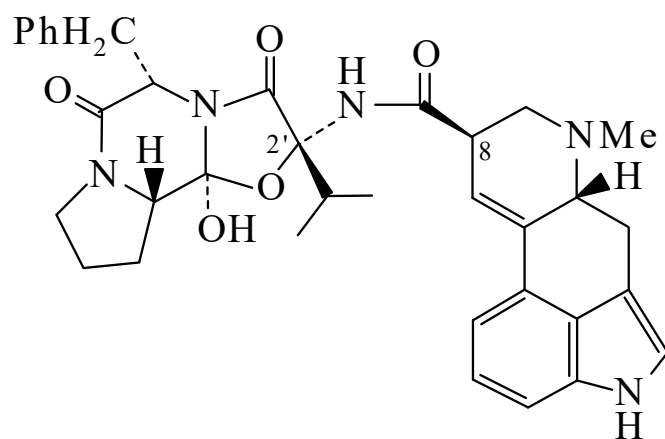




>>Entry Name: Ergocristine

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



Absolute  
configuration

CAS Registry Number: 511-08-0

Related CAS Registry Numbers(s): 8006-25-5 8067-24-1

Molecular Formula: C<sub>35</sub>H<sub>39</sub>N<sub>5</sub>O<sub>5</sub>

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<sub>3</sub>).  $[\alpha]_D -101$  (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<sub>35</sub>H<sub>41</sub>N<sub>5</sub>O<sub>5</sub>

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<sub>35</sub>H<sub>39</sub>N<sub>5</sub>O<sub>5</sub>

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<sub>3</sub>).  $[\alpha]_D^{20} +471$  (c, 0.35 in Py)

Sigma: E6250