ERGOTAMINE

Other names:	Ergotaman-3',6',18-trione, 12'-hydroxy-2'-methyl-5'-(phenylmethyl)-, (5'«alpha»)- Ergotamin (5'«alpha»)-12'-Hydroxy-2'-methyl-5'-(phenylmethyl)ergotoman-3',6',18-trione 12'-Hydroxy-2'-methyl-5'«alpha»-(phenylmethyl)ergotaman-3',6',18-trione Ergoton-A [as succinate]
Inchi:	InChI=1S/C33H35N5O5/c1-32(35-29(39)21-15-23-22-10-6-11-24-28(22)20(17-34-24)16-
InchiKey:	XCGSFFUVFURLIX-UHFFFAOYSA-N
Formula:	C33H35N5O5
SMILES:	CN1CC(C(=O)NC2(C)OC3(O)C4CCCN4C(=O)C(Cc4ccccc4)N3C2=O)C=C2c3cccc4[nH]
Mol. weight [g/mol]:	581.67

Physical Properties

Property code	Value	Unit	Source
ie	7.52	eV	Cheméo Relay (1.0)
logp	1.509		Crippen Method
mcvol	420.900	ml/mol	McGowan Method
rinpol	2366.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C113155&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

ie:	Ionization energy
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices