ERGOCRYPTINE

Other names:	(5'«alpha»)-12'-Hydroxy-2'-(1-methylethyl)-5'-(2-methylpropyl)ergotaman-3',6',18-trione
	12'-Hydroxy-2'-(1-methylethyl)-5'-«alpha»-(2-methylpropyl)ergotaman-3',6',18-trione
	12'-hydroxy-5'«alpha»-isobutyl-2'-isopropylergotaman-3',6',18-trione
	Ergocryptine
	Ergokryptine
	«alpha»-Ergocryptine
	«alpha»-Ergokryptine
Inchi:	InChI=1S/C32H41N5O5/c1-17(2)12-25-29(39)36-11-7-10-26(36)32(41)37(25)30(40)31(4
InchiKey:	YDOTUXAWKBPQJW-UHFFFAOYSA-N
Formula:	C32H41N5O5
SMILES:	CC(C)CC1C(=O)N2CCCC2C2(O)OC(NC(=O)C3C=C4c5cccc6[nH]cc(c56)CC4N(C)C3)(
Mol. weight [g/mol]:	575.71

Physical Properties

Property code	Value	Unit	Source
ie	7.48	eV	Cheméo Relay (1.0)
logp	1.948		Crippen Method
mcvol	430.570	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C511091&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume