

Ergotaman-3',6',18-trione, 12'-hydroxy-2'-(1-methylethyl)-5'-(2-methylpropyl)- (5'«alpha»)-

Other names:	«alpha»-Ergocryptine
	«alpha»-Ergokryptine
	Ergocryptine
	Ergokryptine
	12'-Hydroxy-2'-(1-methylethyl)-5'-«alpha»-(2-methylpropyl)ergotaman-3',6',18-trione
	(5'«alpha»)-12'-Hydroxy-2'-(1-methylethyl)-5'-(2-methylpropyl)ergotaman-3',6',18-trione
	12'-hydroxy-5'«alpha»-isobutyl-2'-isopropylergotaman-3',6',18-trione
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)(C
Mol. weight [g/mol]:	575.70
CAS:	511-09-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.86		Crippen Method
logp	1.948		Crippen Method
mcvol	430.570	ml/mol	McGowan Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C511091&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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