

Dihydroergokryptine

Other names:	Dihydroergocryptine
Inchi:	InChI=1S/C32H43N5O5/c1-17(2)12-25-29(39)36-11-7-10-26(36)32(41)37(25)30(40)31(42)38(43)44
InchiKey:	PBUNVLRHZGSROC-UHFFFAOYSA-N
Formula:	C32H43N5O5
SMILES:	CC(C)CC1C(=O)N2CCCC2C2(O)OC(NC(=O)C3CC4c5cccc6[nH]cc(c56)CC4N(C)C3)(C2)C1
Mol. weight [g/mol]:	577.71
CAS:	76190-07-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.81		Crippen Method
logp	2.039		Crippen Method
mcvol	434.870	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=C76190073&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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<https://www.chemeo.com/cid/77-233-8/Dihydroergokryptine.pdf>

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