

Ergocristine

Other names:	Ergotaman-3',6',18-trione, 12'-hydroxy-2'-(1-methylethyl)-5'-(phenylmethyl)-, (5'«alpha»)-Ergocrystine Ergocristin
Inchi:	InChI=1S/C35H39N5O5/c1-20(2)34(37-31(41)23-16-25-24-11-7-12-26-30(24)22(18-36-2
InchiKey:	HEFIYUQVAZFDEE-UHFFFAOYSA-N
Formula:	C35H39N5O5
SMILES:	CC(C)C1(NC(=O)C2C=C3c4cccc5[nH]cc(c45)CC3N(C)C2)OC2(O)C3CCCN3C(=O)C(C
Mol. weight [g/mol]:	609.71
CAS:	511-08-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.46		Crippen Method
logp	2.145		Crippen Method
mcvol	449.080	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C511080&Units=SI

Legend

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

Latest version available from:
<https://www.chemeo.com/cid/71-028-2/Ergocristine.pdf>

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