

DIHYDROERGOTAMINE

Other names:	Dihydroergotamine Dehydroergotamine DHE 45 Dihydroegotamine Ergotamine, 9,10-dihydro- 9,10-Dihydro-12'-hydroxy-2'-methyl-5'-(phenylmethyl)ergotoman-3',6',18-trione
Inchi:	InChI=1S/C33H37N5O5/c1-32(35-29(39)21-15-23-22-10-6-11-24-28(22)20(17-34-24)16-
InchiKey:	LUZRJRNZXALNLM-UHFFFAOYSA-N
Formula:	C33H37N5O5
SMILES:	CN1CC(C(=O)NC2(C)OC3(O)C4CCCN4C(=O)C(Cc4ccccc4)N3C2=O)CC2c3cccc4[nH]c
Mol. weight [g/mol]:	583.69

Physical Properties

Property code	Value	Unit	Source
logp	1.599		Crippen Method
mcvol	425.200	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C511126&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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