

# Ergotaman-3',6',18-trione, 9,10-dihydro-12'-hydroxy-2'-methyl-5'-(phenylmethyl)- (5'«alpha»,10'«alpha»)-

Other names:	Dihydroergotamine Dehydroergotamine DHE 45 Dihydroergotamine 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]:	583.68
CAS:	511-12-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.81		Crippen Method
logp	1.599		Crippen Method
mcvol	425.200	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C511126&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C511126&amp;Units=SI</a>

## Legend

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

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