Methysergide

Other names:	Ergoline-8-carboxamide, 9,10-didehydro-N-[(S)-1-(hydroxymethyl)propyl]-1,6-dimethyl-, (8«beta»)-
	Ergoline-8«beta»-carboxamide, 9,10-didehydro-N-[1-(hydroxymethyl)propyl]-1,6-dimethyl-
	Deseril
	Desernyl
	Deseryl
	Methyllysergic acid butanolamide
	Methysergid
	(+)-N-[1-(Hydroxymethyl)propyl]-1-methyllysergamide, (D)
	UML 491
	1-Methyl-d-Lysergic acid butanolamide
	1-Methyllysergic acid butanolamide
	Ergoline-8-carboxamide, 9,10-didehydro-N-[1-(hydroxymethyl)propyl]-1,6-dimethyl-, [8«beta»(S)]-
	(+)-9,10-Didehydro-N-[1-(hydroxymethyl)propyl]-1,6-dimethylergoline-8«beta»-carboxami
	(+)-N-[1-(Hydroxymethyl)propyl]-1-methyl-D-lysergamide
	Lysergamide, N-(1-(hydroxymethyl)propyl)-1-methyl-, D-
Inchi:	InChI=1S/C21H27N3O2/c1-4-15(12-25)22-21(26)14-8-17-16-6-5-7-18-20(16)13(10-23(18
InchiKey:	KPJZHOPZRAFDTN-UHFFFAOYSA-N
Formula:	C21H27N3O2
SMILES:	CCC(CO)NC(=O)C1C=C2c3cccc4c3c(cn4C)CC2N(C)C1
Mol. weight [g/mol]:	353.46
CAS:	361-37-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	1.935		Crippen Method
mcvol	279.190	ml/mol	McGowan Method
rinpol	3089.00		NIST Webbook

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=C361375&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
rinpol:	Non-polar retention indices