

Lysergamide

Other names:	Ergoline-8-carboxamide, 9,10-didehydro-6-methyl-, (8«beta»)- Ergine 9,10-Didehydro-6-methyl-ergoline-8-«beta»-carboxamide Lysergic acid amide Lysergic amide (+)-Lysergamide D-Lysergic acid amide Ergoline-8«beta»-carboxamide, 9,10-didehydro-6-methyl-
Inchi:	InChI=1S/C16H17N3O/c1-19-8-10(16(17)20)5-12-11-3-2-4-13-15(11)9(7-18-13)6-14(12)
InchiKey:	GENAHGKEFJLNJB-UHFFFAOYSA-N
Formula:	C16H17N3O
SMILES:	CN1CC(C(N)=O)C=C2c3cccc4[nH]cc(c34)CC21
Mol. weight [g/mol]:	267.33
CAS:	478-94-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	1.041		Crippen Method
mvol	202.870	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C478944&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

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

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