Lysergol

Other names:	Ergoline-8-methanol, 9,10-didehydro-6-methyl-, (8«beta»)- Ergoline-8«beta»-methanol, 9,10-didehydro-6-methyl- Ergoline, 9,10-didehydro-8-hydroxymethyl-6-methyl- Lysergole LOL 9,10-Didehydro-6-methyl-8-hydroxymethylergoline, (8«beta»)- Indolo[4,3-fg]quinoline, ergoline-8-methanol deriv. (6-Methyl-9,10-didehydroergolin-8-yl)methanol-, (8«beta»)- NSC 196867 9,10-didehydro-6-methylergoline-8«beta»-methanol
Inchi:	InChI=1S/C16H18N2O/c1-18-8-10(9-19)5-13-12-3-2-4-14-16(12)11(7-17-14)6-15(13)18/h
InchiKey:	BIXJFIJYBLJTMK-UHFFFAOYSA-N
Formula:	C16H18N2O
SMILES:	CN1CC(CO)C=C2c3cccc4[nH]cc(c34)CC21
Mol. weight [g/mol]:	254.33
CAS:	602-85-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.29		Crippen Method
logp	1.548		Crippen Method
mcvol	197.190	ml/mol	McGowan Method
rinpol	2630.00		NIST Webbook
rinpol	2630.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C602857&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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
rinpol:	Non-polar retention indices