

Ergoline-8-methanol, 8,9-didehydro-6-methyl-

Other names:	Elymoclavin Elymoclavine Elimoclavin Indolo[4,3-fg]quinoline, ergoline-8-methanol deriv.
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/
InchiKey:	DAVNRFCJMIONPO-UHFFFAOYSA-N
Formula:	C16H18N2O
SMILES:	CN1CC(CO)=CC2c3cccc4[nH]cc(c34)CC21
Mol. weight [g/mol]:	254.33
CAS:	548-43-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.33		Crippen Method
logp	1.558		Crippen Method
mcvol	197.190	ml/mol	McGowan Method
rinsol	2784.10		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=C548436&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
rinsol:	Non-polar retention indices

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