Ergoline, 8,9-didehydro-6,8-dimethyl-

Other names:	Ergoline, 8,9-didehydro-6,8-dimethyl-
	8,9-Didehydro-6,8-dimethylergoline
	AGROCLAVIN
	Indolo(4,3-fg)quinoline, 4,6,6a,7,8,10a-hexahydro-7,9-dimethyl-
Inchi:	InChI=1S/C16H18N2/c1-10-6-13-12-4-3-5-14-16(12)11(8-17-14)7-15(13)18(2)9-10/h3-6,8
InchiKey:	XJOOMMHNYOJWCZ-UHFFFAOYSA-N
Formula:	C16H18N2
SMILES:	CC1=CC2c3cccc4[nH]cc(c34)CC2N(C)C1
Mol. weight [g/mol]:	238.33

Physical Properties

Property code	Value	Unit	Source
logp	2.586		Crippen Method
mcvol	191.320	ml/mol	McGowan Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C548425&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices