

Chanoclavine

Other names:	2-Propen-1-ol, 2-methyl-3-[1,3,4,5-tetrahydro-4-(methylamino)benz[cd]indol-5-yl]-, [4R-14«alpha», 5«beta»(E)]-, 6,7-Secoergoline-8-methanol, 8,9-didehydro-6-methyl-, (E)- Chanoclavin-I Chanoclavine I Secaclavin Secaclavine Benz[cd]indole, 2-propen-1-ol deriv. 2-Propen-1-ol, 2-methyl-3-[1,3,4,5-tetrahydro-4«beta»-(methylamino)benz[cd]indol-5«alpha»-yl]-, 2-Methyl-3-[4-(methylamino)-1,3,4,5-tetrahydrobenzo[cd]indol-5-yl]-2-propen-1-ol-, (4R-(4alpha,5beta(E)))
Inchi:	InChI=1S/C16H20N2O/c1-10(9-19)6-13-12-4-3-5-14-16(12)11(8-18-14)7-15(13)17-2/h3-
InchiKey:	SAHHMCVYMGARBT-UXBLZVDNSA-N
Formula:	C16H20N2O
SMILES:	CNC1Cc2c[nH]c3cccc(c23)C1C=C(C)CO
Mol. weight [g/mol]:	256.34
CAS:	2390-99-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	1.852		Crippen Method
mcvol	208.050	ml/mol	McGowan Method
rinpol	2552.90		NIST Webbook
rinpol	2552.90		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2390990&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices

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