

Cinchonan-9-ol, 10,11-dihydro-6'-methoxy-, (8«alpha»,9R)-

Other names:	Dihydroquinine Hydroquinine Quinine, 10,11-dihydro-
Inchi:	InChI=1S/C20H26N2O2/c1-3-13-12-22-9-7-14(13)10-19(22)20(23)16-6-8-21-18-5-4-15(2)
InchiKey:	LJOQGZACKSYWCH-ROBKBVBWSA-N
Formula:	C20H26N2O2
SMILES:	CCC1CN2CCC1CC2C(O)c1ccnc2ccc(OC)cc12
Mol. weight [g/mol]:	326.43
CAS:	522-66-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	3.397		Crippen Method
mcvol	259.420	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C522667&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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