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