Cinchonine

Other names:	Cinchonan-9-ol, (9S)-
	(9S)-Cinchonan-9-ol
	D-Cinchonine
	2-Quinuclidinemethanol, «alpha»-4-quinolyl, 5-vinyl-
Inchi:	InChI=1S/C19H22N2O/c1-2-13-12-21-10-8-14(13)11-18(21)19(22)16-7-9-20-17-6-4-3-5-1
InchiKey:	KMPWYEUPVWOPIM-NAHPKXJFSA-N
Formula:	C19H22N2O
SMILES:	C=CC1CN2CCC1CC2C(O)c1ccnc2ccccc12
Mol. weight [g/mol]:	294.39
CAS:	118-10-5

Physical Properties

Property code	Value	Unit	Source
chs	-10653.00	kJ/mol	NIST Webbook
log10ws	-4.76		Crippen Method
logp	3.165		Crippen Method
mcvol	235.160	ml/mol	McGowan Method
rinpol	2585.00		NIST Webbook
rinpol	2580.00		NIST Webbook
rinpol	2575.00		NIST Webbook
rinpol	2583.00		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=C118105&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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