Quinidine

Other names:	(+)-Quindine
	(+)-Quinidine
	(8R,9S)-6'-Methoxycinchonan-9-ol
	(8R,9S)-Quinidine
	(9S)-6'-Methoxycinchonan-9-ol
	2-Quinuclidinemethanol, «alpha»-(6-methoxy-4-quinolyl)-5-vinyl-
	2-Quinuclidinemethanol, Â«alphaÂ»-(6-methoxy-4-quinolyl)-5-vinyl-
	6'-Methoxycinchonan-9-ol, (8R,9S)-
	6-Methoxy-«alpha»-(5-vinyl-2-quinuclidinyl)-4-quinolinemethanol
	6-Methoxy-Â«alphaÂ»-(5-vinyl-2-quinuclidinyl)-4-quinolinemethanol
	Chinidin
	Cin-quin
	Cinchonan-9-ol, 6'-methoxy-, (9S)-
	Conchinin
	Conchinine
	Conquinine
	Kinidin
	NCI-C56246
	Pitayin
	Pitayine
	Quindine
	Quinine
	«alpha»-(6-Methoxy-4-quinolyl)-5-vinyl-2-quinuclidinemethanol
	«beta»-Quinidine
	«beta»-Quinine
	Â«alphaÂ»-(6-Methoxy-4-quinolyl)-5-vinyl-2-quinuclidinemethanol
	Â«betaÂ»-Quinidine
	Â«betaÂ»-Quinine
Inchi:	InChI=1S/C20H24N2O2/c1-3-13-12-22-9-7-14(13)10-19(22)20(23)16-6-8-21-18-5-4-15(2
InchiKey:	LOUPRKONTZGTKE-WGFDLZGGSA-N
Formula:	C20H24N2O2
SMILES:	C=CC1CN2CCC1CC2C(O)c1ccnc2ccc(OC)cc12
Mol. weight [g/mol]:	324.42
CAS:	56-54-2

Physical Properties

Property code	Value	Unit	Source

chs	-11140.00	kJ/mol	NIST Webbook
chs	-11145.00	kJ/mol	NIST Webbook
log10ws	-2.77		Aqueous Solubility Prediction Method
logp	3.173		Crippen Method
mcvol	255.120	ml/mol	McGowan Method
rinpol	2797.00		NIST Webbook
rinpol	2795.00		NIST Webbook
rinpol	2798.00		NIST Webbook
rinpol	2750.00		NIST Webbook
rinpol	2807.00		NIST Webbook
rinpol	2794.00		NIST Webbook
rinpol	2794.00		NIST Webbook
rinpol	2807.00		NIST Webbook
rinpol	2784.00		NIST Webbook
rinpol	2807.00		NIST Webbook
rinpol	2745.00		NIST Webbook
rinpol	2805.00		NIST Webbook
rinpol	2815.00		NIST Webbook
tf	445.98	K	Aqueous Solubility Prediction Method

Sources

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C56542&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
tf: Normal melting (fusion) point

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