Quinine

Other names:	(-)-Quinine
	(8.alpha.,9R)-6'-methoxycinchonan-9-ol
	(8S,9R)-6'-Methoxycinchonan-9-ol
	(8S,9R)-Quinine
	(R)-(6-methoxyquinolin-4-yl)((1S,2S,4S,5R)-5-vinylquinuclidin-2-yl)methanol
	2-Quinuclidinemethanol, «alpha»-(6-methoxy-4-quinolyl)-5-vinyl-
	2-Quinuclidinemethanol, Â«alphaÂ»-(6-methoxy-4-quinolyl)-5-vinyl-
	6'-Methoxycinchonidine
	6'-Methoxycinchonine
	6-Methoxycinchonine
	Chinin
	Chinine
	Cinchonan-9-ol, 6'-methoxy-, (8alpha,9R)-
	Cinchonan-9-ol, 6'-methoxy-, (8«alpha»,9R)-
	Cinchonan-9-ol, 6'-methoxy-, (8Â«alphaÂ»,9R)-
	NSC 192949
	«alpha»-(6-Methoxy-4-quinolyl)-5-vinyl-2-quinuclidinemethanol
	Â«alphaÂ»-(6-Methoxy-4-quinolyl)-5-vinyl-2-quinuclidinemethanol
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-UHFFFAOYSA-N
Formula:	C20H24N2O2
SMILES:	C=CC1CN2CCC1CC2C(O)c1ccnc2ccc(OC)cc12
Mol. weight [g/mol]:	324.42
CAS:	130-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.79		Aqueous Solubility Prediction Method
logp	3.173		Crippen Method
mcvol	255.120	ml/mol	McGowan Method
rinpol	2773.00		NIST Webbook
rinpol	2820.00		NIST Webbook
rinpol	2796.00		NIST Webbook
rinpol	2760.00		NIST Webbook
rinpol	2825.00		NIST Webbook
rinpol	2820.00		NIST Webbook

rinpol	2755.00	NIST Webbook
rinpol	2797.00	NIST Webbook
rinpol	2773.00	NIST Webbook
rinpol	2815.00	NIST Webbook
rinpol	2800.00	NIST Webbook
rinpol	2798.00	NIST Webbook
rinpol	2803.00	NIST Webbook
rinpol	2755.00	NIST Webbook
rinpol	2825.00	NIST Webbook
rinpol	2797.00	NIST Webbook
rinpol	2797.00	NIST Webbook
rinpol	2803.00	NIST Webbook
rinpol	2815.00	NIST Webbook
rinpol	2797.00	NIST Webbook
rinpol	2798.00	NIST Webbook

Sources

Phase Equilibria of the System Drug + Water:	https://www.doi.org/10.1021/je101163y
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=C130950&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determining the Solubility of Nifedipine and Quinine in Supercritical Fluid Carbon Dioxide Using Continuously Stirred Static Solubility Apparatus Interfaced with Online Supercritical Fluid Chromatography:	https://www.doi.org/10.1021/acs.jced.7b00012

Legend

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