Desethylchloroquine

Other names:	1,4-Pentanediamine, N4-(7-chloro-4-quinolinyl)-N1-ethyl- NSC 13254 Chloroquine M (des-ethyl)
Inchi:	InChI=1S/C16H22ClN3/c1-3-18-9-4-5-12(2)20-15-8-10-19-16-11-13(17)6-7-14(15)16/h6-
InchiKey:	MCYUUUTUAAGOOT-UHFFFAOYSA-N
Formula:	C16H22ClN3
SMILES:	CCNCCCC(C)Nc1ccnc2cc(Cl)ccc12
Mol. weight [g/mol]:	291.82
CAS:	1476-52-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.55		Crippen Method
logp	4.078		Crippen Method
mcvol	235.260	ml/mol	McGowan Method
rinpol	2575.00		NIST Webbook
rinpol	2575.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1476524&Units=SI
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

Legend

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