

Hydroxychloroquine

Other names:	Ethanol, 2-[[4-[(7-chloro-4-quinolinyl)amino]pentyl]ethylamino]- Ethanol, 2-[[4-[(7-chloro-4-quinolyl)amino]pentyl]ethylamino]- Oxychlorochin Plaquenil Quensyl Win 1258-2 WIN 1258 7-Chloro-4-(4-(N-ethyl-N-«beta»-hydroxyethylamino)-1-methylbutylamino)quinoline 7-Chloro-4-(4-(ethyl(2-hydroxyethyl)amino)-1-methylbutylamino)quinoline 7-Chloro-4-(5-(N-ethyl-N-2-hydroxyethylamino)-2-pentyl)aminoquinoline 2-((4-((7-Chloro-4-quinolyl)amino)pentyl)ethylamino)ethanol Oxichloroquine Oxychloroquine (. +/-)-Hydroxychloroquine
Inchi:	InChI=1S/C18H26ClN3O/c1-3-22(11-12-23)10-4-5-14(2)21-17-8-9-20-18-13-15(19)6-7-1
InchiKey:	XXSMGPRMXLTPCZ-UHFFFAOYSA-N
Formula:	C18H26ClN3O
SMILES:	CCN(CCO)CCCC(C)Nc1ccnc2cc(Cl)ccc12
Mol. weight [g/mol]:	335.87
CAS:	118-42-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.03		Crippen Method
logp	3.783		Crippen Method
mcvol	269.310	ml/mol	McGowan Method
rinsol	2872.00		NIST Webbook
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Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C118423&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemo.com/doc/models/crippen_log10ws

Legend

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

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