

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/h6-17

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
rmpol	2575.00		NIST Webbook
rmpol	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/ci9903071>

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

rmpol: Non-polar retention indices

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