Chloroquine

Other names:

1,4-Pentanediamine, N4-(7-chloro-4-quinolinyl)-N1,N1-diethyl-
Quinoline, 7-chloro-4-[[4-(diethylamino)-1-methylbutyl]amino]-
Aralen
Artrichin
Bipiquin
Chloraquine
Chlorochin
Nivaquine B
Quingamine
Reumachlor
Sanoquin
3377 RP
N(sup4)-(7-chloro-4-quinolinyl)-N(sup1),N(sup1)-diethyl-1,4-pentanediamine
Amokin
Arthrochin
Avlochlor
Avloclor
Bemaco
Bemasulph
Benaquin
Chemochin
Chingamin
Chloroquina
Chloroquinium
Chlorquin
Cidanchin
Clorochina
Cocartrit
Dichinalex
Elestol
Gontochin
Heliopar
Imagon
Iroquine
Klorokin
Lapaquin
Malaquin
Malaren
Malarex
Mesylith

Neochin
Nivachine
Nivaquine
Pfizerquine
Quinachlor
Quinagamin
Quinagamine
Quinercyl
Quinilon
Quinoscan
Resochen
Resochin
Resoquina
Reumaquin
Roquine
RP 3377
Silbesan
Siragan
Solprina
Sopaquin
SN 6718
SN 7618
Tresochin
Trochin
W 7618
WIN 244
7-Chloro-4-((4-(diethylamino)-1-methylbutyl)amino)quinoline
Chlorochine
3377 RP opalate
N4-(7-Chloro-4-quinolinyl)-N1,N1-diethyl-1,4-pentanediamine
Capquin
Cloroquine
Ronaquine
(+/-)-Chloroquine

Inchi: InChI=1S/C18H26ClN3/c1-4-22(5-2)12-6-7-14(3)21-17-10-11-20-18-13-15(19)8-9-16(17)

InchiKey: WHTVZRBIWZFKQO-UHFFFAOYSA-N

Formula: C18H26ClN3

SMILES: CCN(CC)CCCC(C)Nc1ccnc2cc(Cl)ccc12

Mol. weight [g/mol]: 319.87

CAS: 54-05-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	4.811		Crippen Method
mcvol	263.440	ml/mol	McGowan Method
rinpol	2630.00		NIST Webbook
rinpol	2600.00		NIST Webbook
rinpol	2590.00		NIST Webbook
rinpol	2660.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C54057&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices