Amodiaquine

Other names:	4-((7-Chloro-4-quinolinyl)amino)-2-((diethylamino)methyl)phenol
	4-((7-Chloro-4-quinolyl)amino)-«alpha»-(diethylamino)-o-cresol
	4-((7-Chloro-4-quinolyl)amino)-Â«alphaÂ»-(diethylamino)-o-cresol
	4-[(7-Chloro-4-quinolinyl)amino]-«alpha»-(diethylamino)-o-cresol
	4-[(7-Chloro-4-quinolinyl)amino]-Â«alphaÂ»-(diethylamino)-o-cresol
	7-Chloro-4-(3-diethylaminomethyl-4-hydroxyanilino)quinoline
	7-Chloro-4-(3-diethylaminomethyl-4-hydroxyphenylamino)quinoline
	Amodiaquin
	Amodiaquine, ring-closed
	CAM-AQ1
	CAM-AQI
	Camochin
	Camoquin
	Camoquinal
	Camoquine
	Flavoquine
	Miaquin
	NSC 13453
	Phenol, 4-[(7-chloro-4-quinolinyl)amino]-2-[(diethylamino)methyl]-
	Quinoline, 7-chloro-4-((3-((diethylamino)methyl)-4-hydroxyphenyl)amino)-
	S. N. 10751
	SN 10,751
	o-Cresol, 4-((7-chloro-4-quinolyl)amino)-«alpha»-(diethylamino)-
	o-Cresol, 4-((7-chloro-4-quinolyl)amino)-Â«alphaÂ»-(diethylamino)-
Inchi:	InChI=1S/C20H22ClN3O/c1-3-24(4-2)13-14-11-16(6-8-20(14)25)23-18-9-10-22-19-12-15
InchiKey:	OVCDSSHSILBFBN-UHFFFAOYSA-N
Formula:	C20H22ClN3O
SMILES:	CCN(CC)Cc1cc(Nc2ccnc3cc(Cl)ccc23)ccc1O
Mol. weight [g/mol]:	355.86
CAS:	86-42-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.79		Aqueous Solubility Prediction Method
logp	5.179		Crippen Method
mcvol	273.730	ml/mol	McGowan Method

tf	433.40	K	Aqueous Solubility Prediction Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86420&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
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
tf:	Normal melting (fusion) point