Primaquine

Other names:	1,4-Pentanediamine, N(4)-(6-methoxy-8-quinolinyl)-
	Neo-Quipenyl
	Primachin
	Quinoline, 8-((4-amino-1-methylbutyl)amino)-6-methoxy-
	S. N. 13272
	SN 13,272
	6-Methoxy-8-((4-amino-1-methylbutyl)amino)quinoline
	8-((4-Amino-1-methylbutyl)amino)-6-methoxyquinoline
	dl-Primaquine
	NSC 27296
	WR 2975
	Primaquin
Inchi:	InChI=1S/C15H21N3O/c1-11(5-3-7-16)18-14-10-13(19-2)9-12-6-4-8-17-15(12)14/h4,6,8-
InchiKey:	INDBQLZJXZLFIT-UHFFFAOYSA-N
Formula:	C15H21N3O
SMILES:	COc1cc(NC(C)CCCN)c2ncccc2c1
Mol. weight [g/mol]:	259.35
CAS:	90-34-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	2.783		Crippen Method
mcvol	214.800	ml/mol	McGowan Method
rinpol	2315.00		NIST Webbook
rinpol	2314.00		NIST Webbook
rinpol	2315.00		NIST Webbook
rinpol	2314.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C90346&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