

Quinisocaine

Other names:	Ethanamine, 2-[(3-butyl-1-isoquinolinyl)oxy]-N,N-dimethyl- Isoquinoline, 3-butyl-1-(2-(dimethylamino)ethoxy)- Chinisocain Dimethisoquin Histaderme Isochinol Prulantex Pruralgan Pruralgin Quinisocain Quinoleine 3-Butyl-1-[2-(dimethylamino)ethoxy]isoquinoline
Inchi:	InChI=1S/C17H24N2O/c1-4-5-9-15-13-14-8-6-7-10-16(14)17(18-15)20-12-11-19(2)3/h6-
InchiKey:	XNMYNYSCEJBRPZ-UHFFFAOYSA-N
Formula:	C17H24N2O
SMILES:	CCCCc1cc2cccc2c(OCCN(C)C)n1
Mol. weight [g/mol]:	272.39
CAS:	86-80-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.63		Crippen Method
logp	3.518		Crippen Method
mcvol	233.000	ml/mol	McGowan Method
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook
rinpol	2030.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86806&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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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