DIMETHISOQUIN

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/h6-8
InchiKey:	XNMYNYSCEJBRPZ-UHFFFAOYSA-N
Formula:	C17H24N2O
SMILES:	CCCCc1cc2ccccc2c(OCCN(C)C)n1
Mol. weight [g/mol]:	272.39

Physical Properties

Property code	Value	Unit	Source
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
tf	337.04	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86806&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point