Dibucaine

Other names:	2-Butoxy-N-(«beta»-diethylaminoethyl)cinchoninamide
	2-Butoxy-N-(Â«betaÂ»-diethylaminoethyl)cinchoninamide
	2-Butoxy-N-[2-(diethylamino)ethyl]cinchoninamide
	2-Butoxyquinoline-4-carboxylic acid diethylaminoethylamide
	2-butoxy-N-(2-diethylaminoethyl)quinoline-4-carboxamide
	4-Quinolinecarboxamide, 2-butoxy-N-[2-(diethylamino)ethyl]-
	Cinchocaine
	Cinchoninamide, 2-butoxy-N-[2-(diethylamino)ethyl]-
	Dermacaine
	Dibucain
	Dibucaine base
	N-[2-(Diethylamino)ethyl]-2-butoxycinchoninamide
	NSC 159055
	Nupercainal
	Nupercaine
	Percamine
	Sovcaine
	«alpha»-Butyloxycinchoninic acid diethylethylenediamide
	Â«alphaÂ»-Butyloxycinchoninic acid diethylethylenediamide
Inchi:	InChI=1S/C20H29N3O2/c1-4-7-14-25-19-15-17(16-10-8-9-11-18(16)22-19)20(24)21-12-1
InchiKey:	PUFQVTATUTYEAL-UHFFFAOYSA-N
Formula:	C20H29N3O2
SMILES:	CCCCOc1cc(C(=O)NCCN(CC)CC)c2ccccc2n1
Mol. weight [g/mol]:	343.46
CAS:	85-79-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Aqueous Solubility Prediction Method
log10ws	-4.39		Aqueous Solubility Prediction Method
logp	3.485		Crippen Method
mcvol	286.820	ml/mol	McGowan Method
rinpol	2701.00		NIST Webbook
rinpol	2740.00		NIST Webbook
rinpol	2706.00		NIST Webbook

rinpol	2677.00		NIST Webbook
rinpol	2693.00		NIST Webbook
rinpol	2693.00		NIST Webbook
rinpol	2690.00		NIST Webbook
rinpol	2675.00		NIST Webbook
tf	337.65	K	Aqueous Solubility Prediction Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C85790&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

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset003.xlsx/351830174/AqueousDa

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

tf: Normal melting (fusion) point