2-BUTOXYQUINOLINE-4-CARBOXYLIC ACID, (2-DIETHYLAMINOETHYL)AMIDE

Other names: 2-Butoxy-N-(«beta»-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
dibucaine
«alpha»-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]: 343.47

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	2706.00		NIST Webbook
rinpol	2740.00		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
rinpol	2701.00		NIST Webbook
tf	337.65	K	Aqueous Solubility Prediction Method

Sources

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

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

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