Doxylamine

Other names:	2-(«alpha»-(2-(Dimethylamino)ethoxy)-«alpha»-methylbenzyl)pyridine
	2-(Â«alphaÂ»-(2-(Dimethylamino)ethoxy)-Â«alphaÂ»-methylbenzyl)pyridine
	Ethanamine, N,N-dimethyl-2-[1-phenyl-1-(2-pyridinyl)ethoxy]-
	N,N-dimethyl-2-(1-phenyl-1-pyridin-2-ylethoxy)ethanamine
	NCI C60684
	Phenyl-2-pyridylmethyl-«beta»-N,N-dimethylaminoethyl ether
	Phenyl-2-pyridylmethyl-Â«betaÂ»-N,N-dimethylaminoethyl ether
	Pyridine, 2-[«alpha»-[2-(dimethylamino)ethoxy]-«alpha»-methylbenzyl]-
	Pyridine, 2-[Â«alphaÂ»-[2-(dimethylamino)ethoxy]-Â«alphaÂ»-methylbenzyl]-
	«alpha»-Dimethylaminoethoxyphenylmethyl-2-picoline
	Â«alphaÂ»-Dimethylaminoethoxyphenylmethyl-2-picoline
Inchi:	InChI=1S/C17H22N2O/c1-17(20-14-13-19(2)3,15-9-5-4-6-10-15)16-11-7-8-12-18-16/h4-1
InchiKey:	HCFDWZZGGLSKEP-UHFFFAOYSA-N
Formula:	C17H22N2O
SMILES:	CN(C)CCOC(C)(c1ccccc1)c1ccccn1
Mol. weight [g/mol]:	270.37
CAS:	469-21-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.82		Aqueous Solubility Prediction Method
logp	2.923		Crippen Method
mcvol	228.700	ml/mol	McGowan Method
rinpol	1945.00		NIST Webbook
rinpol	1925.00		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1958.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1888.00		NIST Webbook
rinpol	1906.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1915.00		NIST Webbook

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C469216&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices