Thonzylamine

Other names:	1,2-Ethanediamine, N-[(4-methoxyphenyl)methyl]-N',N'-dimethyl-N-2-pyrimidinyl- 2-((2-(Dimethylamino)ethyl)(p-methoxybenzyl)amino)pyrimidine 2-[p-Methoxybenzyl-(2-dimethylaminoethyl)amino]pyrimidine Ethylenediamine, N-(p-methoxybenzyl)-N',N'-dimethyl-N-2-pyrimidinyl- N,N-Dimethyl-N'-(p-methoxybenzyl)-N'-(2-pyrimidyl)ethylenediamine N-[(4-methoxyphenyl)methyl]-N',N'-dimethyl-N-pyrimidin-2-ylethane-1,2-diamine NCI-C60708 Neohetramine Pyrimidine, 2-[[2-(dimethylamino)ethyl](p-methoxybenzyl)amino]- Tonzilamine
Inchi:	InChI=1S/C16H22N4O/c1-19(2)11-12-20(16-17-9-4-10-18-16)13-14-5-7-15(21-3)8-6-14/h
InchiKey:	GULNIHOSWFYMRN-UHFFFAOYSA-N
Formula:	C16H22N4O
SMILES:	COc1ccc(CN(CCN(C)C)c2ncccn2)cc1
Mol. weight [g/mol]:	286.37
CAS:	91-85-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.99		Aqueous Solubility Prediction Method
logp	2.053		Crippen Method
mcvol	234.570	ml/mol	McGowan Method
rinpol	2200.00		NIST Webbook
rinpol	2215.00		NIST Webbook
rinpol	2172.00		NIST Webbook
rinpol	2210.00		NIST Webbook
rinpol	2203.00		NIST Webbook
rinpol	2203.00		NIST Webbook
ripol	3095.00		NIST Webbook
ripol	3095.00		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=C91850&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
ripol:	Polar retention indices