Chloropyramine

Other names:	1,2-Ethanediamine, N-[(4-chlorophenyl)methyl]-N',N'-dimethyl-N-2-pyridinyl- p-Chlorbenzyl-«alpha»-pyridyl-dimethyl-aethylendiamin Allergan S Anaphylline Avapena Chlorneoantergan Chloropyribenzamine Chlorpyramine Ethylenediamine, N-(p-chlorobenzyl)-N',N'-dimethyl-N-(2-pyridyl)- Halopyramine N-(p-Chlorobenzyl)-N',N'-dimethyl-N-(2-pyridyl)ethylenediamine Pyridine, 2-((p-chlorobenzyl)(2-(dimethylamino)ethyl)amino)- Suprastin Synopen Synopen R Synpen 2-((p-Chlorobenzyl)(2-(dimethylamino)ethyl)amino)pyridine Chloroneoantergan NSC 241038
Inchi:	InChI=1S/C16H20ClN3/c1-19(2)11-12-20(16-5-3-4-10-18-16)13-14-6-8-15(17)9-7-14/h3-
InchiKey:	ICKFFNBDFNZJSX-UHFFFAOYSA-N
Formula:	C16H20ClN3
SMILES:	CN(C)CCN(Cc1ccc(Cl)cc1)c1ccccn1
Mol. weight [g/mol]:	289.80
CAS:	59-32-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.77		Crippen Method
logp	3.303		Crippen Method
mcvol	230.960	ml/mol	McGowan Method
rinpol	2180.00		NIST Webbook
rinpol	2230.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2190.00		NIST Webbook
rinpol	2234.00		NIST Webbook
rinpol	2234.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59325&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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