Brompheniramine

Other names:	2-Pyridinepropanamine, «gamma»-(4-bromophenyl)-N,N-dimethyl- Pyridine, 2-[p-bromo-«alpha»-[2-(dimethylamino)ethyl]benzyl]- Bromopheniramine Ilvin Parabromdylamine Parabromodylamine 2-[p-Bromo-«alpha»-[2-(dimethylamino)ethyl]benzyl]pyridine 3-(4-Bromophenyl)-N,N-dimethyl-3-(2-pyridinyl)-1-propanamine 1-(p-Bromophenyl)-1-(2-pyridyl)-3-dimethylaminopropane 3-(p-Bromophenyl)-3-(2-pyridyl)-N,N-dimethylpropylamine
Inchi:	InChI=1S/C16H19BrN2/c1-19(2)12-10-15(16-5-3-4-11-18-16)13-6-8-14(17)9-7-13/h3-9,1
InchiKey:	ZDIGNSYAACHWNL-UHFFFAOYSA-N
Formula:	C16H19BrN2
SMILES:	CN(C)CCC(c1ccc(Br)cc1)c1ccccn1
Mol. weight [g/mol]:	319.24
CAS:	86-22-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.71		Crippen Method
logp	3.928		Crippen Method
mcvol	226.240	ml/mol	McGowan Method
rinpol	2090.00		NIST Webbook
rinpol	2158.80		NIST Webbook
rinpol	2095.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2082.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2100.00		NIST Webbook
rinpol	2105.00		NIST Webbook
rinpol	2080.00		NIST Webbook
rinpol	2115.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2096.00		NIST Webbook
rinpol	2075.00		NIST Webbook
rinpol	2067.00		NIST Webbook
rinpol	2105.00		NIST Webbook

rinpol	2109.00	NIST Webbook
rinpol	2096.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C132218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

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