Pheniramine

Other names:	3-Phenyl-3-(2-pyridyl)-N,N-dimethylpropylamine 2-Pyridinepropanamine, N,N-dimethyl-«gamma»-phenyl- Pyridine, 2-[«alpha»-[2-(dimethylamino)ethyl]benzyl]- Feniramine Prophenpyridamine Pyriton Trimeton Tripoton 2-[«alpha»-[2-(Dimethylamino)ethyl]benzyl]pyridine N,N-Dimethyl-3-phenyl-3-(2-pyridyl)propylamine 1-Phenyl-1-(2-pyridyl)-3-dimethylaminopropane 2-(3-Dimethylamino-1-phenylpropyl)pyridine NCI-C60695 Propheniramine Pyridine, 2[alpha-(2-dimethylaminoethyl)benzyl] NSC 47965
Inchi:	InChI=1S/C16H20N2/c1-18(2)13-11-15(14-8-4-3-5-9-14)16-10-6-7-12-17-16/h3-10,12,15
InchiKey:	IJHNSHDBIRRJRN-UHFFFAOYSA-N
Formula:	C16H20N2
SMILES:	CN(C)CCC(c1ccccc1)c1ccccn1
Mol. weight [g/mol]:	240.34
CAS:	86-21-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.55		Crippen Method
logp	3.165		Crippen Method
mcvol	208.740	ml/mol	McGowan Method
rinpol	1805.00		NIST Webbook
rinpol	1779.00		NIST Webbook
rinpol	1810.00		NIST Webbook
rinpol	1820.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1805.00		NIST Webbook
rinpol	1799.00		NIST Webbook
rinpol	1840.00		NIST Webbook
rinpol	1802.00		NIST Webbook

rinpol	1788.00	NIST Webbook
rinpol	1788.00	NIST Webbook
rinpol	1779.00	NIST Webbook
rinpol	1805.00	NIST Webbook
rinpol	1804.00	NIST Webbook
rinpol	1779.00	NIST Webbook
rinpol	1804.00	NIST Webbook
rinpol	1810.00	NIST Webbook
ripol	2469.00	NIST Webbook
ripol	2469.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C86215&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

ripol: Polar retention indices