

Methapyrilene

Other names:	1,2-Ethanediamine, N,N-dimethyl-N'-2-pyridinyl-N'-(2-thienylmethyl)-2-[[2-(Dimethylamino)ethyl]-2-thenylamino]pyridine A 3322 AH-42 Histadryl Lulamin Metapyrilene Methapyrilene N,N-Dimethyl-N'-2-pyridinyl-N'-(2-thienylmethyl)-1,2-ethanediamine N,N-Dimethyl-N'-pyrid-2-yl-N'-2-thenylethylenediamine N-(«alpha»-Pyridyl)-N-(«alpha»-thenyl)-N',N'-dimethylethylenediamine NCI-C55550 Paradormalene Pyrathyn Pyridine, 2-[[2-(dimethylamino)ethyl]-2-thenylamino]- Pyrinistab Pyrinistol Rcra waste number U155 Rest-On Restryl Semikon Sleepwell Tenalin Thenylene Thenylpyramine Thionylan
Inchi:	InChI=1S/C14H19N3S/c1-16(2)9-10-17(12-13-6-5-11-18-13)14-7-3-4-8-15-14/h3-8,11H,9
InchiKey:	HNJJXZKZRAWDPF-UHFFFAOYSA-N
Formula:	C14H19N3S
SMILES:	CN(C)CCN(Cc1cccs1)c1cccn1
Mol. weight [g/mol]:	261.39
CAS:	91-80-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Aqueous Solubility Prediction Method

logp	2.711		Crippen Method
mcvol	211.190	ml/mol	McGowan Method
rinpol	1975.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1985.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1980.00		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	334.85		NIST Webbook
rinpol	337.56		NIST Webbook
rinpol	339.60		NIST Webbook
rinpol	1965.00		NIST Webbook
rinpol	334.85		NIST Webbook
rinpol	1994.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1981.00		NIST Webbook
rinpol	339.60		NIST Webbook
rinpol	1980.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C91805&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Legend

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

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