Thenyldiamine

Other names:	1,2-Ethanediamine, N,N-dimethyl-N'-2-pyridinyl-N'-(3-thienylmethyl)-
	Pyridine, 2-[[2-(dimethylamino)ethyl]-3-thenylamino]-
	Dethlandiamine
	Dethylandiamine
	Tenfidil
	Thefanil
	Thenfadil
	Thenyldiamine (pharmaceutical)
	WIN 2848
	2-[(2-Dimethylaminoethyl)-3-thenylamino]pyridine
	N-(2-Dimethylaminoethyl)-N-2-pyridyl-3-thenylamine
	N-(«alpha»-Pyridyl)-N-(«beta»-thenyl)-N',N'-dimethylethylenediamine
	NCI-C60640
Inchi:	InChI=1S/C14H19N3S/c1-16(2)8-9-17(11-13-6-10-18-12-13)14-5-3-4-7-15-14/h3-7,10,12
InchiKey:	RCGYDFVCAAKKNG-UHFFFAOYSA-N
Formula:	C14H19N3S
SMILES:	CN(C)CCN(Cc1ccsc1)c1ccccn1
Mol. weight [g/mol]:	261.39
CAS:	91-79-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.84		Crippen Method
logp	2.711		Crippen Method
mcvol	211.190	ml/mol	McGowan Method
rinpol	1963.00		NIST Webbook
rinpol	2005.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1963.00		NIST Webbook
rinpol	2008.00		NIST Webbook
rinpol	1992.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C91792&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

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