Thenalidine

Other names:	4-Piperidinamine, 1-methyl-N-phenyl-N-(2-thienylmethyl)-
	Piperidine, 1-methyl-4-(N-2-thenylanilino)-
	1-Methyl-4-amino-N-phenyl-N-(2-thenyl)piperidine
	1-Methyl-4-N-2-thenylanilinopiperidine
	Thenophenopiperidine
	Sandostene
	Thenaldine
	Sanbosten
Inchi:	InChI=1S/C17H22N2S/c1-18-11-9-16(10-12-18)19(14-17-8-5-13-20-17)15-6-3-2-4-7-15/h
InchiKey:	KLOHYVOVXOUKQI-UHFFFAOYSA-N
Formula:	C17H22N2S
SMILES:	CN1CCC(N(Cc2cccs2)c2ccccc2)CC1
Mol. weight [g/mol]:	286.44
CAS:	86-12-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.92		Crippen Method
logp	3.849		Crippen Method
mcvol	232.620	ml/mol	McGowan Method
rinpol	2252.00		NIST Webbook
rinpol	2270.00		NIST Webbook
rinpol	2260.00		NIST Webbook
rinpol	2270.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C86124&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