Chlorothen

Other names:	1,2-Ethanediamine, N-[(5-chloro-2-thienyl)methyl]-N',N'-dimethyl-N-2-pyridinyl- Pyridine, 2-[(5-chloro-2-thenyl)[2-(dimethylamino)ethyl]amino]- Chloromethapyrilene Chloropyrilene Chlorothenylpyramine Chlorthenylpyramine Histachlorylene Pyrithen Tagathen 2-((5-Chloro-2-thenyl)(2-dimethylaminoethyl)amino)pyridine N,N-Dimethyl-N'-(2-pyridyl)-N'-(5-chloro-2-thenyl)ethylenediamine Ethylenediamine, N-(5-chloro-2-thenyl)-N',N'-dimethyl-N-2-pyridyl- NCI-C60559 2-Thenylamine, 5-chloro-N-(2-(dimethylamino)ethyl)-N-2-pyridyl-
Inchi:	InChI=1S/C14H18ClN3S/c1-17(2)9-10-18(14-5-3-4-8-16-14)11-12-6-7-13(15)19-12/h3-8
InchiKey:	XAEXSWVTEJHRMH-UHFFFAOYSA-N
Formula:	C14H18ClN3S
SMILES:	CN(C)CCN(Cc1ccc(Cl)s1)c1ccccn1
Mol. weight [g/mol]:	295.83
CAS:	148-65-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.52		Crippen Method
logp	3.365		Crippen Method
mcvol	223.430	ml/mol	McGowan Method
rinpol	2153.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2133.00		NIST Webbook
rinpol	2120.00		NIST Webbook
rinpol	2133.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C148652&Units=SI

Legend

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