Ethylmethylthiambutene

Other names:	3-Buten-2-amine, N-ethyl-N-methyl-4,4-di-2-thienyl- Allylamine, N-ethyl-N,1-dimethyl-3,3-di-2-thienyl- Emethibutin NIH 5145 1-C50 2-Propenamine, N-Ethyl-N,1-dimethyl-3,3-di-2-thienyl- 3-Ethylmethylamino-1,1-di-(2'-thienyl)-1-butene Ethylmethiambutene N-Ethyl-N-methyl-4,4-di(2-thienyl)-3-buten-2-amine N-Ethyl-N,1-dimethyl-3,3-di-2-thienylallylamine
Inchi:	InChI=1S/C15H19NS2/c1-4-16(3)12(2)11-13(14-7-5-9-17-14)15-8-6-10-18-15/h5-12H,4H
InchiKey:	MORSAEFGQPDBKM-UHFFFAOYSA-N
Formula:	C15H19NS2
SMILES:	CCN(C)C(C)C=C(c1cccs1)c1cccs1
Mol. weight [g/mol]:	277.45
CAS:	441-61-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.30		Crippen Method
logp	4.582		Crippen Method
mcvol	221.670	ml/mol	McGowan Method
rinpol	1943.00		NIST Webbook
rinpol	1943.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C441612&Units=SI
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

Legend

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