

# 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
rmpol	1943.00		NIST Webbook
rmpol	1943.00		NIST Webbook

## Sources

**Crippen Method:**

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

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C441612&Units=SI>

# Legend

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

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