Thiambutene

Other names:	3-Buten-2-amine, N,N-diethyl-4,4-di-2-thienyl-
	Allylamine, N,N-diethyl-1-methyl-3,3-di-2-thienyl-
	Allylamine, N,N-diethyl-3,3-di-2-thienyl-1-methyl-
	Diethylthiambutene
	191C49
	Diethibutin
	3-Diethylamino-1,1-bis(2-thienyl)-1-butene
	3-Diethylamino-1,1-dithienylbut-1-ene
	3-Diethylamino-1,1-di(2'-thienyl)-1-butene
	3-Diethylamino-1,1-di(2'-thienyl)but-1-ene
	N,N-Diethyl-1-methyl-3,3-di-2-thienylallylamine
	NIH-4185
	Themalon
Inchi:	InChI=1S/C16H21NS2/c1-4-17(5-2)13(3)12-14(15-8-6-10-18-15)16-9-7-11-19-16/h6-13H
InchiKey:	CBYWMRHUUVRIAF-UHFFFAOYSA-N
Formula:	C16H21NS2
SMILES:	CCN(CC)C(C)C=C(c1cccs1)c1cccs1
Mol. weight [g/mol]:	291.48
CAS:	86-14-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.72		Crippen Method
logp	4.972		Crippen Method
mcvol	235.760	ml/mol	McGowan Method
rinpol	2008.00		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=C86146&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