Dimethylthiambutene

Other names:	3-Buten-2-amine, N,N-dimethyl-4,4-di-2-thienyl-
	Allylamine, N,N,1-trimethyl-3,3-di-2-thienyl-
	Dimethibutin
	Ohton
	338C48
	Allylamine, 3,3-di-2-thienyl-N,N,1-trimethyl-
	3-Dimethylamino-1,1-bis(2-thienyl)-1-butene
	3-Dimethylamino-1,1-di-(2'-thienyl)-1-butene
	3-Dimethylamino-1,1-di-(2'-thienyl)but-1-ene
	N,N,1-Trimethyl-3,3-di-2-thienylallylamine
	N,N,1-Trimethyl-3,3-di(2-thienyl)-2-propenylamine
	Aminobutene
	Kobaton
	NIH-4542
	Takaton
Inchi:	InChI=1S/C14H17NS2/c1-11(15(2)3)10-12(13-6-4-8-16-13)14-7-5-9-17-14/h4-11H,1-3H3
InchiKey:	CANBGVXYBPOLRR-UHFFFAOYSA-N
Formula:	C14H17NS2
SMILES:	CC(C=C(c1cccs1)c1cccs1)N(C)C
Mol. weight [g/mol]:	263.42
CAS:	524-84-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.88		Crippen Method
logp	4.191		Crippen Method
mcvol	207.580	ml/mol	McGowan Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C524845&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