3-Buten-2-amine, N,N-dimethyl-4,4-di-2-thienyl-

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]: 263.43

Physical Properties

Property code	Value	Unit	Source
hvap	79.70	kJ/mol	Cheméo Relay (1.0)
ie	7.84	eV	Cheméo Relay (1.0)
logp	4.191		Crippen Method
mcvol	207.580	ml/mol	McGowan Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook
tb	610.33	K	Cheméo Relay (1.0)
tf	351.60	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C524845&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	

Legend

hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point