

5'-methyl-5-(3-buten-1-ynyl)-2,2'-bithienyl

Inchi:	InChI=1S/C13H10S2/c1-3-4-5-11-7-9-13(15-11)12-8-6-10(2)14-12/h3,6-9H,1H2,2H3
InchiKey:	OZUJLEZCMIGWSN-UHFFFAOYSA-N
Formula:	C13H10S2
SMILES:	C=CC#Cc1ccc(-c2ccc(C)s2)s1
Mol. weight [g/mol]:	230.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Crippen Method
logp	4.323		Crippen Method
mcvol	174.910	ml/mol	McGowan Method
rinpol	1992.00		NIST Webbook
rinpol	1992.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R401815&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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

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