

5-methylaceto-5'-(3-buten-1-ynil)-2,2'-bithienyl

Inchi:	InChI=1S/C15H12OS2/c1-3-4-5-12-6-8-14(17-12)15-9-7-13(18-15)10-11(2)16/h3,6-9H,1
InchiKey:	YINMMFXHFCEWCK-UHFFFAOYSA-N
Formula:	C15H12OS2
SMILES:	C=CC#Cc1ccc(-c2ccc(CC(C)=O)s2)s1
Mol. weight [g/mol]:	272.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	4.146		Crippen Method
mcvol	204.660	ml/mol	McGowan Method
rinpol	2373.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R503976&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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