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

Inchi: InChI=1S/C15H12O2S2/c1-3-4-5-12-6-8-14(18-12)15-9-7-13(19-15)10-17-11(2)16/h3,6-9
InchiKey: SYEWLUATUDURPR-UHFFFAOYSA-N
Formula: C15H12O2S2
SMILES: C=CC#Cc1ccc(-c2ccc(COC(C)=O)s2)s1
Mol. weight [g/mol]: 288.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.56		Crippen Method
logp	4.077		Crippen Method
mcvol	210.530	ml/mol	McGowan Method
rinpol	2443.00		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=R587865&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