5-(3,4-Diacetoxy-1-butenynyl)-2,2'-bithienyl

Inchi: InChI=1S/C16H14O4S2/c1-11(17)19-10-13(20-12(2)18)5-6-14-7-8-16(22-14)15-4-3-9-21
InchiKey: RGIIXLVKXLFDLP-UHFFFAOYSA-N
Formula: C16H14O4S2
SMILES: CC(=O)OCC(C#Cc1ccc(-c2cccs2)s1)OC(C)=O
Mol. weight [g/mol]: 334.41
CAS: 1233-95-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	3.323		Crippen Method
mcvol	236.360	ml/mol	McGowan Method
rinpol	2598.20		NIST Webbook
rinpol	2591.00		NIST Webbook
rinpol	2591.00		NIST Webbook
rinpol	2598.20		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=C1233950&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