4-(2,2'-Bithiophen-5-yl)but-3-yn-1-yl acetate

Inchi: InChI=1S/C14H12O2S2/c1-11(15)16-9-3-2-5-12-7-8-14(18-12)13-6-4-10-17-13/h4,6-8,10
InchiKey: KHPAKGUGOFYJNA-UHFFFAOYSA-N
Formula: C14H12O2S2
SMILES: CC(=O)OCCC#Cc1ccc(-c2cccs2)s1
Mol. weight [g/mol]: 276.37
CAS: 1219-28-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.83		Crippen Method
logp	3.781		Crippen Method
mcvol	200.740	ml/mol	McGowan Method
rinpol	2356.40		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2356.40		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1219289&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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