

# 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/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](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

Latest version available from:

<https://www.cheméo.com/cid/115-861-8/4-2-2-Bithiophen-5-yl-but-3-yn-1-yl-acetate.pdf>

Generated by Cheméo on 2024-04-30 19:58:48.50132637 +0000 UTC m=+16796377.421903683.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.