

# 5-(Pent-3-en-1-yn-1-yl)-2,2'-bithiophene

<b>Inchi:</b>	InChI=1S/C13H10S2/c1-2-3-4-6-11-8-9-13(15-11)12-7-5-10-14-12/h2-3,5,7-10H,1H3/b3-
<b>InchiKey:</b>	FEESEVYIPPQXKI-NSCUHMNNSA-N
<b>Formula:</b>	C13H10S2
<b>SMILES:</b>	CC=CC#Cc1ccc(-c2cccs2)s1
<b>Mol. weight [g/mol]:</b>	230.35
<b>CAS:</b>	129050-92-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	4.404		Crippen Method
mcvol	174.910	ml/mol	McGowan Method
rinpol	2093.90		NIST Webbook
rinpol	2093.90		NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C129050926&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C129050926&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/83-123-3/5-Pent-3-en-1-yn-1-yl-2-2-bithiophene.pdf>

Generated by Cheméo on 2024-04-23 13:49:30.05030492 +0000 UTC m=+16169418.970882236.

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