5-[(3Z)-Pent-3-en-1-yn-1-yl]-2,2'-bithiophene

Inchi: 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-
InchiKey: FEESEVYIPPQXKI-IHWYPQMZSA-N
Formula: C13H10S2
SMILES: CC=CC#Cc1ccc(-c2cccs2)s1
Mol. weight [g/mol]: 230.35

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	2046.30		NIST Webbook
rinpol	2046.30		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U415023&Units=SI

Legend

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

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