5-(1-pentynyl)-2,2'-bithienyl

Inchi: InChI=1S/C13H12S2/c1-2-3-4-6-11-8-9-13(15-11)12-7-5-10-14-12/h5,7-10H,2-3H2,1H3
InchiKey: JWUFYYYJQPWOHO-UHFFFAOYSA-N
Formula: C13H12S2
SMILES: CCCC#Cc1ccc(-c2cccs2)s1
Mol. weight [g/mol]: 232.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.54		Crippen Method
logp	4.628		Crippen Method
mcvol	179.210	ml/mol	McGowan Method
rinpol	2043.00		NIST Webbook
rinpol	2043.00		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=R401820&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

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