5-(3-buten-1-ynyl)-2,2'-bithienyl

Inchi: InChI=1S/C12H8S2/c1-2-3-5-10-7-8-12(14-10)11-6-4-9-13-11/h2,4,6-9H,1H2
InchiKey: GWAIEOFEEWQORO-UHFFFAOYSA-N
Formula: C12H8S2
SMILES: C=CC#Cc1ccc(-c2cccs2)s1
Mol. weight [g/mol]: 216.32
CAS: 1134-61-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.98		Crippen Method
logp	4.014		Crippen Method
mcvol	160.820	ml/mol	McGowan Method
rinpol	1892.00		NIST Webbook
rinpol	1935.10		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1935.10		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=C1134618&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