Methyl 3,4-dimethyl-2-thienyl disulfide

Inchi: InChI=1S/C7H10S2/c1-5-4-9-7(8-3)6(5)2/h4H,1-3H3
InchiKey: XHHSQVPPAQTZFT-UHFFFAOYSA-N
Formula: C7H10S2
SMILES: CSc1scc(C)c1C
Mol. weight [g/mol]: 158.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	3.087		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
rinpol	1460.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1514.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R56884&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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