propyl 3,4-dimethyl-2-thienyl disulfide

Inchi: InChI=1S/C9H14S3/c1-4-5-11-12-9-8(3)7(2)6-10-9/h6H,4-5H2,1-3H3
InchiKey: GQTMTKKPPSGWKQ-UHFFFAOYSA-N
Formula: C9H14S3
SMILES: CCCSSc1scc(C)c1C
Mol. weight [g/mol]: 218.40
CAS: 126876-33-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	4.515		Crippen Method
mcvol	167.260	ml/mol	McGowan Method
rinpol	1663.80		NIST Webbook
rinpol	1635.00		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=C126876333&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