3,4-Dimethyl-2-(propyldisulfanyl)thiophene

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]: 218.41

Physical Properties

Property code	Value	Unit	Source
logp	4.515		Crippen Method
mcvol	167.260	ml/mol	McGowan Method
rinpol	1635.00		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1663.80		NIST Webbook
rinpol	1635.00		NIST Webbook
rinpol	1663.80		NIST Webbook

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C126876333&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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