3,4-dimethyl-2-(methyldisulfanyl)thiophene

Inchi: InChI=1S/C7H10S3/c1-5-4-9-7(6(5)2)10-8-3/h4H,1-3H3
InchiKey: RGPFFCJRZNZZJL-UHFFFAOYSA-N
Formula: C7H10S3
SMILES: CSSc1scc(C)c1C
Mol. weight [g/mol]: 190.35
CAS: 126876-26-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	3.735		Crippen Method
mcvol	139.080	ml/mol	McGowan Method
rinpol	1500.20		NIST Webbook
rinpol	1500.20		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C126876264&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