(E)-3,4-Dimethyl-2-(prop-1-en-1-yldisulfanyl)thiopl

Inchi: InChI=1S/C9H12S3/c1-4-5-11-12-9-8(3)7(2)6-10-9/h4-6H,1-3H3/b5-4+
InchiKey: KNLAYDMFHCJZFB-SNAWJCMRSA-N
Formula: C9H12S3
SMILES: CC=CSSc1scc(C)c1C
Mol. weight [g/mol]: 216.39
CAS: 153001-05-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.98		Crippen Method
logp	4.639		Crippen Method
mcvol	162.960	ml/mol	McGowan Method
rinpol	1671.10		NIST Webbook
rinpol	1671.10		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C153001059&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