2,3-Dihydro-5-methyl-4-[(2-methyl-3-furyl)dithio]fu

Other names: (2-Methylfuryl-3)-(2-methyl-4,5-dihydrofuryl) disulfide
Inchi: InChI=1S/C10H12O2S2/c1-7-9(3-5-11-7)13-14-10-4-6-12-8(10)2/h3,5H,4,6H2,1-2H3
InchiKey: XHMKUMOVGFTUCW-UHFFFAOYSA-N
Formula: C10H12O2S2
SMILES: CC1=C(SSc2ccoc2C)CCO1
Mol. weight [g/mol]: 228.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.80		Crippen Method
logp	3.980		Crippen Method
mcvol	161.580	ml/mol	McGowan Method
rinpol	1587.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1544.00		NIST Webbook
rinpol	1587.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U365973&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

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