2-(2-methyl-3-furanyldithio)pentan-3-one

Inchi: InChI=1S/C11H16O2S2/c1-4-5-10(12)9(3)14-15-11-6-7-13-8(11)2/h6-7,9H,4-5H2,1-3H3
InchiKey: ZHBZBRISXANORO-UHFFFAOYSA-N
Formula: C11H16O2S2
SMILES: CCCC(=O)C(C)SSc1ccoc1C
Mol. weight [g/mol]: 244.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.78		Crippen Method
logp	4.086		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
rinpol	1593.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R180424&Units=SI

Legend

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