3-[2-Methyl-(3-thienyldithio)]butan-2-one

Inchi: InChI=1S/C9H12OS3/c1-6(10)7(2)12-13-9-4-5-11-8(9)3/h4-5,7H,1-3H3
InchiKey: YXEGLEYEOHTHJV-UHFFFAOYSA-N
Formula: C9H12OS3
SMILES: CC(=O)C(C)SSc1ccsc1C
Mol. weight [g/mol]: 232.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.97		Crippen Method
logp	3.774		Crippen Method
mcvol	168.830	ml/mol	McGowan Method
rinpol	1711.00		NIST Webbook

Sources

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=R90608&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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