3-(3-Thienyldithio)butan-2-one

Inchi: InChI=1S/C8H10OS3/c1-6(9)7(2)11-12-8-3-4-10-5-8/h3-5,7H,1-2H3
InchiKey: DBSAPEBQSUTLOA-UHFFFAOYSA-N
Formula: C8H10OS3
SMILES: CC(=O)C(C)SSc1ccsc1
Mol. weight [g/mol]: 218.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	3.466		Crippen Method
mcvol	154.740	ml/mol	McGowan Method
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R90630&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.