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

Inchi: InChI=1S/C10H14OS3/c1-4-9(11)7(2)13-14-10-5-6-12-8(10)3/h5-7H,4H2,1-3H3
InchiKey: PGDWEJUJUYDSMI-UHFFFAOYSA-N
Formula: C10H14OS3
SMILES: CCC(=O)C(C)SSc1ccsc1C
Mol. weight [g/mol]: 246.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	4.164		Crippen Method
mcvol	182.920	ml/mol	McGowan Method
rinpol	1795.00		NIST Webbook
rinpol	1795.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R90466&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

Latest version available from:
https://www.chemeo.com/cid/83-373-6/2-2-Methyl-3-thienyldithio-pentan-3-one.pdf
Generated by Cheméo on 2024-10-12 07:50:17.461682359 +0000 UTC m=+3300280.098651608.

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