2-[(2-furylmethyl)dithio]-3-pentanone

Inchi: InChI=1S/C10H14O2S2/c1-3-10(11)8(2)14-13-7-9-5-4-6-12-9/h4-6,8H,3,7H2,1-2H3
InchiKey: YWUGFXRRVFFUFD-UHFFFAOYSA-N
Formula: C10H14O2S2
SMILES: CCC(=O)C(C)SSCc1ccco1
Mol. weight [g/mol]: 230.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.33		Crippen Method
logp	3.529		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
rinpol	1686.00		NIST Webbook
rinpol	1686.00		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=R223006&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

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