2-methyl-3-furyl 2-oxo-3-pentyl disulfide

Other names: 2-Pentanone, 3-(2-methyl-3-furyldithio)
Inchi: InChI=1S/C10H14O2S2/c1-4-9(7(2)11)13-14-10-5-6-12-8(10)3/h5-6,9H,4H2,1-3H3
InchiKey: HUNHUMWMMZADPP-UHFFFAOYSA-N
Formula: C10H14O2S2
SMILES: CCC(SSc1ccoc1C)C(C)=O
Mol. weight [g/mol]: 230.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.37		Crippen Method
logp	3.696		Crippen Method
mcvol	172.440	ml/mol	McGowan Method
rinpol	1571.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1574.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1557.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	1557.00		NIST Webbook
ripol	2205.00		NIST Webbook
ripol	2145.00		NIST Webbook
ripol	2145.00		NIST Webbook
ripol	2205.00		NIST Webbook
ripol	2145.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U365958&Units=SI
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

Legend

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

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