1-[(2-methylL-3-furyl)dithio]-2-propanone

Other names: 2-Propanone, 1-(2-methyl-3-furyldithio)
Inchi: InChI=1S/C8H10O2S2/c1-6(9)5-11-12-8-3-4-10-7(8)2/h3-4H,5H2,1-2H3
InchiKey: FAADBRMWDANEGB-UHFFFAOYSA-N
Formula: C8H10O2S2
SMILES: CC(=O)CSSc1ccoc1C
Mol. weight [g/mol]: 202.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.42		Crippen Method
logp	2.917		Crippen Method
mcvol	144.260	ml/mol	McGowan Method
rinpol	1476.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1462.00		NIST Webbook
rinpol	1476.00		NIST Webbook
rinpol	1445.00		NIST Webbook
rinpol	1462.00		NIST Webbook
ripol	2235.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2200.00		NIST Webbook
ripol	2235.00		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=U357166&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
ripol:	Polar retention indices