

1-[2-Methyl-(3-furyldithio)]butan-2-one

Inchi:	InChI=1S/C9H12O2S2/c1-3-8(10)6-12-13-9-4-5-11-7(9)2/h4-5H,3,6H2,1-2H3
InchiKey:	PJSTYLQHOBXNFN-UHFFFAOYSA-N
Formula:	C9H12O2S2
SMILES:	CCC(=O)CSSc1ccoc1C
Mol. weight [g/mol]:	216.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.83		Crippen Method
logp	3.307		Crippen Method
mcvol	158.350	ml/mol	McGowan Method
rinpol	1572.00		NIST Webbook

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R90402&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

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