

2-(2-methyl-3-furanyldithio)pentan-3-one

Inchi:	InChI=1S/C11H16O2S2/c1-4-5-10(12)9(3)14-15-11-6-7-13-8(11)2/h6-7,9H,4-5H2,1-3H3
InchiKey:	ZHBZBRISXANORO-UHFFFAOYSA-N
Formula:	C11H16O2S2
SMILES:	CCCC(=O)C(C)SSc1ccoc1C
Mol. weight [g/mol]:	244.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.78		Crippen Method
logp	4.086		Crippen Method
mcvol	186.530	ml/mol	McGowan Method
rinpola	1593.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R180424&Units=SI

Legend

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

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