

2-methyl-3-(2-methyl-3-furanyldithio)thiophene

Inchi: InChI=1S/C10H10OS3/c1-8-10(4-6-12-8)14-13-7-9-3-2-5-11-9/h2-6H,7H2,1H3
InchiKey: FJPMJBNIIFQDQK-UHFFFAOYSA-N
Formula: C10H10OS3
SMILES: Cc1sccc1SSCc1ccc1
Mol. weight [g/mol]: 242.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.17		Crippen Method
logp	4.590		Crippen Method
mcvol	167.760	ml/mol	McGowan Method
rinpol	1727.00		NIST Webbook

Sources

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=R180444&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/56-296-2/2-methyl-3-2-methyl-3-furanyldithio-thiophene.pdf>

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