2-methyl-3-furyl 3-thienyl disulphide

Other names: (2-methyl-3-furanyl) (3-thienyl) disulfide
Inchi: InChI=1S/C9H8OS3/c1-7-9(2-4-10-7)13-12-8-3-5-11-6-8/h2-6H,1H3
InchiKey: AKUXGGSFKSEULP-UHFFFAOYSA-N
Formula: C9H8OS3
SMILES: Cc1occc1SSc1ccsc1
Mol. weight [g/mol]: 228.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.73		Crippen Method
logp	4.449		Crippen Method
mcvol	153.670	ml/mol	McGowan Method
rinpol	1716.00		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=R189332&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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