Furylmethyl 2-methyl-3-furyl disulfide

Inchi: InChI=1S/C9H8O2S2/c1-2-8(11-4-1)7-12-13-9-3-5-10-6-9/h1-6H,7H2
InchiKey: IOILHFACDQBYGN-UHFFFAOYSA-N
Formula: C9H8O2S2
SMILES: c1coc(CSSc2ccoc2)c1
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.67		Crippen Method
logp	3.813		Crippen Method
mcvol	143.190	ml/mol	McGowan Method
rinpol	1548.00		NIST Webbook
rinpol	1548.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R78979&Units=SI
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

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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