

(2-Methylfuryl-3-)-(2-methyldihydrofuryl-3-) disulfide

Inchi: InChI=1S/C10H12O2S2/c1-7-9(3-5-11-7)13-14-10-4-6-12-8(10)2/h3-7,9H,1-2H3
InchiKey: PLRVTMPWGHHRQMF-UHFFFAOYSA-N
Formula: C10H12O2S2
SMILES: Cc1occc1SSC1C=COC1C
Mol. weight [g/mol]: 228.33

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.53		Crippen Method
logp	3.629		Crippen Method
mcvol	161.580	ml/mol	McGowan Method
rinsol	1538.00		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.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=R125843&Units=SI>

Legend

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

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