(2-furfuryl)-(1-(2'-furyl)-1-ethyl) disulfide

Inchi: InChI=1S/C11H12O2S2/c1-9(11-5-3-7-13-11)15-14-8-10-4-2-6-12-10/h2-7,9H,8H2,1H3
InchiKey: NTRHPKKYOZDMGL-UHFFFAOYSA-N
Formula: C11H12O2S2
SMILES: CC(SSCc1ccco1)c1ccco1
Mol. weight [g/mol]: 240.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.49		Crippen Method
logp	4.515		Crippen Method
mcvol	171.370	ml/mol	McGowan Method
rinpol	1696.00		NIST Webbook
rinpol	1696.00		NIST Webbook
ripol	2449.00		NIST Webbook
ripol	2449.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R225597&Units=SI

Legend

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