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

Inchi: InChI=1S/C12H14O2S2/c1-9(11-5-3-7-13-11)15-16-10(2)12-6-4-8-14-12/h3-10H,1-2H3
InchiKey: NECWWEQOLRUBBE-UHFFFAOYSA-N
Formula: C12H14O2S2
SMILES: CC(SSC(C)c1ccco1)c1ccco1
Mol. weight [g/mol]: 254.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.87		Crippen Method
logp	5.076		Crippen Method
mcvol	185.460	ml/mol	McGowan Method
rinpol	1732.00		NIST Webbook
rinpol	1732.00		NIST Webbook
ripol	2422.00		NIST Webbook
ripol	2422.00		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=R225646&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
ripol: Polar retention indices