2-furfuryl 2-thienylmethyl disulfide

Inchi: InChI=1S/C10H10OS3/c1-3-9(11-5-1)7-13-14-8-10-4-2-6-12-10/h1-6H,7-8H2
InchiKey: OARWODBXQRECEZ-UHFFFAOYSA-N
Formula: C10H10OS3
SMILES: c1coc(CSSCc2cccs2)c1
Mol. weight [g/mol]: 242.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.13		Crippen Method
logp	4.423		Crippen Method
mcvol	167.760	ml/mol	McGowan Method
rinpol	1820.00		NIST Webbook
rinpol	1820.00		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=R219908&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.