2-furfuryl 2-thienyl trisulfide

Inchi: InChI=1S/C9H8OS4/c1-3-8(10-5-1)7-12-14-13-9-4-2-6-11-9/h1-6H,7H2
InchiKey: PCNRBTKPEIVRND-UHFFFAOYSA-N
Formula: C9H8OS4
SMILES: c1coc(CSSSc2cccs2)c1
Mol. weight [g/mol]: 260.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.56		Crippen Method
logp	4.930		Crippen Method
mcvol	170.020	ml/mol	McGowan Method
rinpol	1964.00		NIST Webbook
rinpol	1964.00		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=R219913&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.