di-2-furfuryl trisulfide

Other names: bis(2-furylmethyl)trisulfide
Inchi: InChI=1S/C10H10O2S3/c1-3-9(11-5-1)7-13-15-14-8-10-4-2-6-12-10/h1-6H,7-8H2
InchiKey: XPRPVIPSHWDFBI-UHFFFAOYSA-N
Formula: C10H10O2S3
SMILES: c1coc(CSSSCc2ccco2)c1
Mol. weight [g/mol]: 258.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-13.98		Crippen Method
logp	4.602		Crippen Method
mcvol	173.630	ml/mol	McGowan Method
rinpol	1879.00		NIST Webbook
rinpol	1901.00		NIST Webbook
rinpol	1901.00		NIST Webbook
rinpol	1879.00		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=R220007&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