bis(2-methyl-3-furyl) disulfide

Inchi: InChI=1S/C9H8O2S2/c1-7-9(3-5-11-7)13-12-8-2-4-10-6-8/h2-6H,1H3
InchiKey: ZZONAHHQTRFZLU-UHFFFAOYSA-N
Formula: C9H8O2S2
SMILES: Cc1occc1SSc1ccoc1
Mol. weight [g/mol]: 212.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.70		Crippen Method
logp	3.980		Crippen Method
mcvol	143.190	ml/mol	McGowan Method
rinpol	1520.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1526.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1534.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1494.00		NIST Webbook
rinpol	1527.00		NIST Webbook
rinpol	1530.00		NIST Webbook
rinpol	1543.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1537.00		NIST Webbook
rinpol	1547.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1508.00		NIST Webbook
rinpol	1542.00		NIST Webbook
ripol	2141.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2100.00		NIST Webbook
ripol	2150.00		NIST Webbook
ripol	2153.00		NIST Webbook
ripol	2151.00		NIST Webbook
ripol	2156.00		NIST Webbook
ripol	2150.00		NIST Webbook

ripol	2145.00	NIST Webbook
ripol	2127.00	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=R69671&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