

bis(2-methyl-3-thienyl) disulfide

Other names: bis-(2-Methylthienyl-3-) disulfide
Inchi: InChI=1S/C10H10S4/c1-7-9(3-5-11-7)13-14-10-4-6-12-8(10)2/h3-6H,1-2H3
InchiKey: ZFCWB IQPXUGVGV-UHFFFAOYSA-N
Formula: C10H10S4
SMILES: Cc1sccc1SSc1ccsc1C
Mol. weight [g/mol]: 258.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.23		Crippen Method
logp	5.226		Crippen Method
mcvol	178.240	ml/mol	McGowan Method
rinpol	1855.00		NIST Webbook
rinpol	1868.00		NIST Webbook
rinpol	1840.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U365968&Units=SI>
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>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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