

2-furfuryl 2-thienyl disulfide

Other names: 2-furylmethyl 2-thienyl disulphide
Inchi: InChI=1S/C9H8OS3/c1-3-8(10-5-1)7-12-13-9-4-2-6-11-9/h1-6H,7H2
InchiKey: ZOAPZVMUVRMPMN-UHFFFAOYSA-N
Formula: C9H8OS3
SMILES: c1coc(CSSc2cccs2)c1
Mol. weight [g/mol]: 228.35

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.69		Crippen Method
logp	4.282		Crippen Method
mcvol	153.670	ml/mol	McGowan Method
rinpol	1736.00		NIST Webbook
rinpol	1736.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R189258&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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