

Methyl 2,4-dimethyl-3-thienyl disulfide

Inchi:	InChI=1S/C7H10S2/c1-5-4-9-6(2)7(5)8-3/h4H,1-3H3
InchiKey:	JSZKVFVTHOTPGU-UHFFFAOYSA-N
Formula:	C7H10S2
SMILES:	CSc1c(C)csc1C
Mol. weight [g/mol]:	158.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	3.087		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
rinsol	1440.00		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=R56870&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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<https://www.chemeo.com/cid/29-827-2/Methyl-2-4-dimethyl-3-thienyl-disulfide.pdf>

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