

2-methyl-3-methyltrithiofuran

Inchi: InChI=1S/C6H8OS3/c1-5-6(3-4-7-5)9-10-8-2/h3-4H,1-2H3
InchiKey: UJSUGHKPAPNABI-UHFFFAOYSA-N
Formula: C6H8OS3
SMILES: CSSSc1ccoc1C
Mol. weight [g/mol]: 192.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.17		Crippen Method
logp	3.606		Crippen Method
mcpvol	130.860	ml/mol	McGowan Method
ripol	1383.00		NIST Webbook
ripol	1392.00		NIST Webbook
ripol	1383.00		NIST Webbook
ripol	1945.00		NIST Webbook
ripol	1976.00		NIST Webbook
ripol	1979.00		NIST Webbook
ripol	1969.00		NIST Webbook
ripol	1945.00		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=R230163&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
rinpol: Non-polar retention indices
ripol: Polar retention indices

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