

2,5-dimethyl-3-(methyldithio)furan

Inchi: InChI=1S/C7H10OS2/c1-5-4-7(10-9-3)6(2)8-5/h4H,1-3H3
InchiKey: ZZXDUGZYDILQMO-UHFFFAOYSA-N
Formula: C7H10OS2
SMILES: CSSc1cc(C)oc1C
Mol. weight [g/mol]: 174.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.77		Crippen Method
logp	3.267		Crippen Method
mcvol	128.600	ml/mol	McGowan Method
ripol	1762.00		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=R489751&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
ripol: Polar retention indices

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