

Thiophene, 3,5-dimethyl-2-(methylthio)-

Other names: 3,5-Dimethyl-2-(methylthio)thiophene
Inchi: InChI=1S/C7H10S2/c1-5-4-6(2)9-7(5)8-3/h4H,1-3H3
InchiKey: NCWOSJBAFGDYEH-UHFFFAOYSA-N
Formula: C7H10S2
SMILES: CSc1sc(C)cc1C
Mol. weight [g/mol]: 158.28
CAS: 69442-33-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.92		Crippen Method
logp	3.087		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
rinpol	1259.20		NIST Webbook
rinpol	1230.00		NIST Webbook
rinpol	1259.20		NIST Webbook
rinpol	1230.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C69442337&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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