

2-Methylthieno[2,3-b]thiophene

Inchi: InChI=1S/C7H6S2/c1-5-4-6-2-3-8-7(6)9-5/h2-4H,1H3
InchiKey: CKDAPMQEHBEIBW-UHFFFAOYSA-N
Formula: C7H6S2
SMILES: Cc1cc2ccsc2s1
Mol. weight [g/mol]: 154.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	3.271		Crippen Method
mcvol	107.570	ml/mol	McGowan Method
rinpol	1306.00		NIST Webbook
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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=R640352&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

Latest version available from:

<https://www.chemeo.com/cid/92-831-7/2-Methylthieno-2-3-b-thiophene.pdf>

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