

Thieno[2,3-b]thiophene,2-methyl-

Inchi: InChI=1S/C7H6S2/c1-5-4-7-6(9-5)2-3-8-7/h2-4H,1H3
InchiKey: REF XKVVKFBUOND-UHFFFAOYSA-N
Formula: C7H6S2
SMILES: Cc1cc2sccc2s1
Mol. weight [g/mol]: 154.25
CAS: 13393-75-4

Physical Properties

Property code	Value	Unit	Source
ie	8.12	eV	NIST Webbook
log10ws	-3.27		Crippen Method
logp	3.271		Crippen Method
mcvol	107.570	ml/mol	McGowan Method
rinpol	1364.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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=C13393754&Units=SI>

Legend

ie: Ionization energy
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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