

Thiophene, 3-propylthio

Inchi: InChI=1S/C7H10S2/c1-2-4-9-7-3-5-8-6-7/h3,5-6H,2,4H2,1H3
InchiKey: JZKOZBMAZVCPX-UHFFFAOYSA-N
Formula: C7H10S2
SMILES: CCCSc1ccsc1
Mol. weight [g/mol]: 158.28

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.81		Crippen Method
logp	3.250		Crippen Method
mcvol	122.730	ml/mol	McGowan Method
rinpol	1224.00		NIST Webbook
rinpol	1229.00		NIST Webbook
rinpol	1213.00		NIST Webbook
rinpol	1220.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1234.00		NIST Webbook
rinpol	1224.00		NIST Webbook
rinpol	1218.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R57804&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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