

Thiophene, 3,5-dimethyl-2-propyl

Other names: 3,5-Dimethyl-2-propylthiophene
Inchi: InChI=1S/C9H14S/c1-4-5-9-7(2)6-8(3)10-9/h6H,4-5H2,1-3H3
InchiKey: AIKMKEMIIQNNNSI-UHFFFAOYSA-N
Formula: C9H14S
SMILES: CCCc1sc(C)cc1C
Mol. weight [g/mol]: 154.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	3.317		Crippen Method
mcvol	134.560	ml/mol	McGowan Method
rinpol	1129.00		NIST Webbook
rinpol	1131.00		NIST Webbook
rinpol	1129.00		NIST Webbook
rinpol	1132.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R41879&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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