3,5-Dimethyl-2-propylthiophene

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: AIKMKEMIIQNNSI-UHFFFAOYSA-N
Formula: C9H14S
SMILES: CCCc1sc(C)cc1C
Mol. weight [g/mol]: 154.28

Physical Properties

Property code	Value	Unit	Source
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
rinpol	1129.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R41879&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices