2,3-Dimethyl-5-propylthiophene

Other names: 2,3-Dimethyl-5-propylthiophene
Inchi: InChI=1S/C9H14S/c1-4-5-9-6-7(2)8(3)10-9/h6H,4-5H2,1-3H3
InchiKey: SSPQIAIXQRRLGU-UHFFFAOYSA-N
Formula: C9H14S
SMILES: CCCc1cc(C)c(C)s1
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	1142.00		NIST Webbook
rinpol	1144.00		NIST Webbook
rinpol	1142.00		NIST Webbook
rinpol	1144.00		NIST Webbook
tb	471.68	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=R41730&Units=SI

Legend

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

tb: Normal Boiling Point Temperature