

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

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