

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/ci990307I

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/34-206-5/3-5-Dimethyl-2-propylthiophene.pdf>

Generated by Cheméo on 2026-07-21 10:17:48.355161552 +0000 UTC m=+140164.197046950.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.