4-methyl-2-ethyl-5-propylthiazole

Inchi: InChI=1S/C9H15NS/c1-4-6-8-7(3)10-9(5-2)11-8/h4-6H2,1-3H3
InchiKey: SRVOSKQWHYHPGF-UHFFFAOYSA-N
Formula: C9H15NS
SMILES: CCCc1sc(CC)nc1C
Mol. weight [g/mol]: 169.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.49		Crippen Method
logp	2.966		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinpol	1224.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R217393&Units=SI

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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