

5-Ethyl-2-isopropyl-4-methyl-thiazole

Other names: 2-isopropyl-4-methyl-5-ethyl thiazole
Inchi: InChI=1S/C9H15NS/c1-5-8-7(4)10-9(11-8)6(2)3/h6H,5H2,1-4H3
InchiKey: AYEGWZGUAQDVNB-UHFFFAOYSA-N
Formula: C9H15NS
SMILES: CCc1sc(C(C)C)nc1C
Mol. weight [g/mol]: 169.29

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.46		Crippen Method
logp	3.137		Crippen Method
mcvol	144.540	ml/mol	McGowan Method
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook
rinpol	1179.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R308677&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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