

2-butyl-5-ethyl-4-methyl-thiazole

Inchi: InChI=1S/C10H17NS/c1-4-6-7-10-11-8(3)9(5-2)12-10/h4-7H2,1-3H3
InchiKey: DLQAOPSTXFKJFN-UHFFFAOYSA-N
Formula: C10H17NS
SMILES: CCCCc1nc(C)c(CC)s1
Mol. weight [g/mol]: 183.31

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.91		Crippen Method
logp	3.357		Crippen Method
mcvol	158.630	ml/mol	McGowan Method
rinpol	1356.00		NIST Webbook
rinpol	1356.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R497559&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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<https://www.chemeo.com/cid/19-945-2/2-butyl-5-ethyl-4-methyl-thiazole.pdf>

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