

# 4,5-dimethyl-2-nonyl-thiazole

<b>Inchi:</b>	InChI=1S/C14H25NS/c1-4-5-6-7-8-9-10-11-14-15-12(2)13(3)16-14/h4-11H2,1-3H3
<b>InchiKey:</b>	TUBGURMWJWGLPY-UHFFFAOYSA-N
<b>Formula:</b>	C14H25NS
<b>SMILES:</b>	CCCCCCCCc1nc(C)c(C)s1
<b>Mol. weight [g/mol]:</b>	239.42

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.68		Crippen Method
logp	5.053		Crippen Method
mcvol	214.990	ml/mol	McGowan Method
rinpola	1795.00		NIST Webbook

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R497777&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R497777&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpola:</b>	Non-polar retention indices

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