

# Thiazole, 2-methyl-4-propyl-

<b>Other names:</b>	2-Methyl-4-propylthiazole
<b>Inchi:</b>	InChI=1S/C7H11NS/c1-3-4-7-5-9-6(2)8-7/h5H,3-4H2,1-2H3
<b>InchiKey:</b>	KPTRSWJGYUCLLM-UHFFFAOYSA-N
<b>Formula:</b>	C7H11NS
<b>SMILES:</b>	CCc1csc(C)n1
<b>Mol. weight [g/mol]:</b>	141.23
<b>CAS:</b>	41981-63-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.69		Crippen Method
logp	2.404		Crippen Method
mcvol	116.360	ml/mol	McGowan Method
rinpol	1085.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1068.00		NIST Webbook
ripol	1428.00		NIST Webbook
ripol	1428.00		NIST Webbook

## Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C41981639&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C41981639&amp;Units=SI</a>

## Legend

<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume  
**rinpol:** Non-polar retention indices  
**ripol:** Polar retention indices

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