

# Thiazole, 2-butyl-4-methyl-

<b>Other names:</b>	2-n-Butyl-4-methylthiazole 2-butyl-4-methyl-thiazole
<b>Inchi:</b>	InChI=1S/C8H13NS/c1-3-4-5-8-9-7(2)6-10-8/h6H,3-5H2,1-2H3
<b>InchiKey:</b>	HVRMJTCTZVGJDO-UHFFFAOYSA-N
<b>Formula:</b>	C8H13NS
<b>SMILES:</b>	CCCCc1nc(C)cs1
<b>Mol. weight [g/mol]:</b>	155.26
<b>CAS:</b>	76572-47-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	2.794		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
rinpol	1141.00		NIST Webbook
rinpol	1222.00		NIST Webbook
rinpol	1141.00		NIST Webbook
ripol	1500.00		NIST Webbook

## Sources

<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=C76572479&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C76572479&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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

**rinpol:** Non-polar retention indices

**ripol:** Polar retention indices

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