

# Thiazole, 4-methyl-2-(2-methylpropyl)-

<b>Other names:</b>	2-iso-Butyl-4-methylthiazole Thiazole, 2-isobutyl-4-methyl
<b>Inchi:</b>	InChI=1S/C8H13NS/c1-6(2)4-8-9-7(3)5-10-8/h5-6H,4H2,1-3H3
<b>InchiKey:</b>	JBUCYVMFLWLDIO-UHFFFAOYSA-N
<b>Formula:</b>	C8H13NS
<b>SMILES:</b>	Cc1csc(CC(C)C)n1
<b>Mol. weight [g/mol]:</b>	155.26
<b>CAS:</b>	61323-24-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.87		Crippen Method
logp	2.650		Crippen Method
mcvol	130.450	ml/mol	McGowan Method
rinpol	1086.00		NIST Webbook
rinpol	1086.00		NIST Webbook
ripol	1420.00		NIST Webbook
ripol	1420.00		NIST Webbook

## Sources

<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=C61323248&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C61323248&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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