

# 4-Thiazolecarboxamide, 5-amino-2-methylthio-

<b>Inchi:</b>	InChI=1S/C5H7N3OS2/c1-10-5-8-2(3(6)9)4(7)11-5/h7H2,1H3,(H2,6,9)
<b>InchiKey:</b>	ZGYKQSVGGNYQKY-UHFFFAOYSA-N
<b>Formula:</b>	C5H7N3OS2
<b>SMILES:</b>	CSc1nc(C(N)=O)c(N)s1
<b>Mol. weight [g/mol]:</b>	189.26
<b>CAS:</b>	52868-69-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.54		Crippen Method
logp	0.546		Crippen Method
mcvol	126.060	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C52868696&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C52868696&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>
<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

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