

# 3-Anilinomethyl-2(3)-benzole thiazolethione

<b>Inchi:</b>	InChI=1S/C14H12N2S2/c17-14-16(10-15-11-6-2-1-3-7-11)12-8-4-5-9-13(12)18-14/h1-9,1
<b>InchiKey:</b>	ILQSOMABDWQHPR-UHFFFAOYSA-N
<b>Formula:</b>	C14H12N2S2
<b>SMILES:</b>	S=c1sc2ccccc2n1CNc1ccccc1
<b>Mol. weight [g/mol]:</b>	272.39
<b>CAS:</b>	5392-35-8

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.46		Crippen Method
logp	4.502		Crippen Method
mcvol	198.100	ml/mol	McGowan Method

## 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=C5392358&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5392358&amp;Units=SI</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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