

# Thiadiazole, 2-anilino-5-mercapto-1,3,4-

<b>Other names:</b>	5-anilino-1,3,4-thiadiazole-2(3H)-thione
<b>Inchi:</b>	InChI=1S/C8H7N3S2/c12-8-11-10-7(13-8)9-6-4-2-1-3-5-6/h1-5H,(H,9,10)(H,11,12)
<b>InchiKey:</b>	BOJLJKMUGYYKCZ-UHFFFAOYSA-N
<b>Formula:</b>	C8H7N3S2
<b>SMILES:</b>	Sc1nnc(Nc2ccccc2)s1
<b>Mol. weight [g/mol]:</b>	209.29
<b>CAS:</b>	10253-83-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.08		Crippen Method
logp	2.570		Crippen Method
mcvol	143.000	ml/mol	McGowan Method

## 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=C10253835&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C10253835&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

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