

# 5-Phenyl-1,2,3,4-thiatriazole

<b>Other names:</b>	Phenyl-1,2,3,4-thiatriazol
<b>Inchi:</b>	InChI=1S/C7H5N3S/c1-2-4-6(5-3-1)7-8-9-10-11-7/h1-5H
<b>InchiKey:</b>	PXZQTGLTLYTSHC-UHFFFAOYSA-N
<b>Formula:</b>	C7H5N3S
<b>SMILES:</b>	<chem>c1ccc(-c2nnns2)cc1</chem>
<b>Mol. weight [g/mol]:</b>	163.20
<b>CAS:</b>	34733-85-2

## Physical Properties

Property code	Value	Unit	Source
ie	9.10	eV	NIST Webbook
log10ws	-3.13		Crippen Method
logp	1.600		Crippen Method
mcvol	112.560	ml/mol	McGowan Method

## 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=C34733852&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C34733852&amp;Units=SI</a>
<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>

## Legend

<b>ie:</b>	Ionization energy
<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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<https://www.chemeo.com/cid/55-746-3/5-Phenyl-1-2-3-4-thiatriazole.pdf>

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