

# 2-(2-Benzothiazolyl)-5-methoxyphenol

<b>Inchi:</b>	InChI=1S/C14H11NO2S/c1-17-9-6-7-10(12(16)8-9)14-15-11-4-2-3-5-13(11)18-14/h2-8,10
<b>InchiKey:</b>	KQUJPMLQKNTPL-UHFFFAOYSA-N
<b>Formula:</b>	C14H11NO2S
<b>SMILES:</b>	COc1ccc(-c2nc3ccccc3s2)c(O)c1
<b>Mol. weight [g/mol]:</b>	257.31
<b>CAS:</b>	90481-46-2

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.07		Crippen Method
logp	3.677		Crippen Method
mcvol	183.510	ml/mol	McGowan Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C90481462&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C90481462&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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