

# 2,5-Dimethylbenzoxazole

<b>Other names:</b>	Benzoxazole, 2,5-dimethyl-
<b>Inchi:</b>	InChI=1S/C9H9NO/c1-6-3-4-9-8(5-6)10-7(2)11-9/h3-5H,1-2H3
<b>InchiKey:</b>	XVQGFGKAPKEUFT-UHFFFAOYSA-N
<b>Formula:</b>	C9H9NO
<b>SMILES:</b>	Cc1ccc2oc(C)nc2c1
<b>Mol. weight [g/mol]:</b>	147.17
<b>CAS:</b>	5676-58-4

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.73		Crippen Method
logp	2.445		Crippen Method
mcvol	114.600	ml/mol	McGowan Method
tb	491.70	K	NIST Webbook

## 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=C5676584&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5676584&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>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>tb:</b>	Normal Boiling Point Temperature

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