

# 1H-Benzotriazole, 5-methyl-

<b>Other names:</b>	Tolutriazole 5-Methyl-1,2,3-benzotriazole 5-Methylbenzotriazole 5-Methyl-1H-benzotriazole 5-Methyl-1H-benzo-1,2,3-triazole 1H-Benzotriazole, 6-methyl- 5-Tolyltriazole 6-Methyl-1,2,3-benzotriazole NSC 122012 6-methylbenzotriazole
<b>Inchi:</b>	InChI=1S/C7H7N3/c1-5-2-3-6-7(4-5)9-10-8-6/h2-4H,1H3,(H,8,9,10)
<b>InchiKey:</b>	LRUDIIUSNGCQKF-UHFFFAOYSA-N
<b>Formula:</b>	C7H7N3
<b>SMILES:</b>	Cc1ccc2[nH]nnc2c1
<b>Mol. weight [g/mol]:</b>	133.15
<b>CAS:</b>	136-85-6

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.50		Crippen Method
logp	0.784		Crippen Method
mcvol	100.510	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=C136856&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C136856&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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