

5,6-Dimethyl-1H-benzotriazole

Other names:	5,6-Dimethylbenzotriazole 1H-Benzotriazole, 5,6-dimethyl-
Inchi:	InChI=1S/C8H9N3/c1-5-3-7-8(4-6(5)2)10-11-9-7/h3-4H,1-2H3,(H,9,10,11)
InchiKey:	MVPKIPGHRNIOPT-UHFFFAOYSA-N
Formula:	C8H9N3
SMILES:	Cc1cc2nn[nH]c2cc1C
Mol. weight [g/mol]:	147.18
CAS:	4184-79-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.98		Crippen Method
logp	1.093		Crippen Method
mcvol	114.600	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4184796&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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