1H-Benzotriazole, 1-methyl-

Other names:	1-Methyl-1,2,3-benzotriazole
	1-Methylbenzotriazole
	1-Methyl-1H-benzotriazole
Inchi:	InChI=1S/C7H7N3/c1-10-7-5-3-2-4-6(7)8-9-10/h2-5H,1H3
InchiKey:	HXQHRUJXQJEGER-UHFFFAOYSA-N
Formula:	C7H7N3
SMILES:	Cn1nnc2ccccc21
Mol. weight [g/mol]:	133.15
CAS:	13351-73-0

Physical Properties

Property code	Value	Unit	Source
affp	931.20	kJ/mol	NIST Webbook
basg	898.70	kJ/mol	NIST Webbook
log10ws	-4.10		Crippen Method
logp	0.968		Crippen Method
mcvol	100.510	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C13351730&Units=SI

Legend

affp:	Proton affinity
basg:	Gas basicity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume