

2H-Benzotriazole, 2-methyl-

Other names:	2-Methylbenzotriazole 2-Methyl-2H-benzotriazole
Inchi:	InChI=1S/C7H7N3/c1-10-8-6-4-2-3-5-7(6)9-10/h2-5H,1H3
InchiKey:	PWORFEDVDWBHSJ-UHFFFAOYSA-N
Formula:	C7H7N3
SMILES:	Cn1nc2ccccc2n1
Mol. weight [g/mol]:	133.15
CAS:	16584-00-2

Physical Properties

Property code	Value	Unit	Source
affp	890.10	kJ/mol	NIST Webbook
basg	855.90	kJ/mol	NIST Webbook
ie	8.54	eV	NIST Webbook
log10ws	-4.10		Crippen Method
logp	0.968		Crippen Method
mcvol	100.510	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16584002&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

affp:	Proton affinity
basg:	Gas basicity
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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