

4H-1,2,4-Triazole, 4-methyl-

Other names:	4-Methyl-1,2,4-triazole 4-Methyl-4H-1,2,4-triazole
Inchi:	InChI=1S/C3H5N3/c1-6-2-4-5-3-6/h2-3H,1H3
InchiKey:	XILPCSMEKCBYFO-UHFFFAOYSA-N
Formula:	C3H5N3
SMILES:	Cn1cnnc1
Mol. weight [g/mol]:	83.09
CAS:	10570-40-8

Physical Properties

Property code	Value	Unit	Source
ie	9.30	eV	NIST Webbook
log10ws	-2.29		Crippen Method
logp	-0.185		Crippen Method
mcvol	63.610	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=C10570408&Units=SI

Legend

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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