1-Methyl-1H-1,2,4-triazole

Other names: 1-Methyl-1,2,4-triazole
1H-1,2,4-Triazole, 1-methyl-
Inchi: InChI=1S/C3H5N3/c1-6-3-4-2-5-6/h2-3H,1H3
InchiKey: MWZDIEIXRBWPLG-UHFFFAOYSA-N
Formula: C3H5N3
SMILES: Cn1cncn1
Mol. weight [g/mol]: 83.09
CAS: 6086-21-1

Physical Properties

Property code	Value	Unit	Source
ie	9.80	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/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=C6086211&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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