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

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

Physical Properties

Property code	Value	Unit	Source
ie	9.80	eV	NIST Webbook
logp	-0.185		Crippen Method
mcvol	63.610	ml/mol	McGowan Method

Sources

Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C6086211&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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