

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/ci990307I>

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/25-489-2/1H-1-2-4-Triazole-1-methyl.pdf>

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