

# 1H-1,2,4-Triazole, 3-chloro-

<b>Other names:</b>	s-Triazole, 3-chloro- 3-Chloro-s-triazole 3-Chloro-1H-1,2,4-triazole 1H-1,2,4-Triazole, 5-chloro-
<b>Inchi:</b>	InChI=1S/C2H2ClN3/c3-2-4-1-5-6-2/h1H,(H,4,5,6)
<b>InchiKey:</b>	QGOUKZPSCTVYLX-UHFFFAOYSA-N
<b>Formula:</b>	C2H2ClN3
<b>SMILES:</b>	Clc1nc[nH]n1
<b>Mol. weight [g/mol]:</b>	103.51
<b>CAS:</b>	6818-99-1

## Physical Properties

Property code	Value	Unit	Source
ie	10.10	eV	NIST Webbook
log10ws	-0.91		Crippen Method
logp	-0.024		Crippen Method
mcvol	61.760	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C6818991&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6818991&amp;Units=SI</a>

## Legend

<b>ie:</b>	Ionization energy
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume

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