

# 5-Carboxy-1,2,3-triazole

<b>Other names:</b>	4-Carboxy-1,2,3-triazole
<b>Inchi:</b>	InChI=1S/C3H3N3O2/c7-3(8)2-1-4-6-5-2/h1H,(H,7,8)(H,4,5,6)
<b>InchiKey:</b>	GTODOEDLCLNTSLG-UHFFFAOYSA-N
<b>Formula:</b>	C3H3N3O2
<b>SMILES:</b>	O=C(O)c1cnn[nH]1
<b>Mol. weight [g/mol]:</b>	113.07
<b>CAS:</b>	16681-70-2

## Physical Properties

Property code	Value	Unit	Source
chs	-1364.00	kJ/mol	NIST Webbook
log10ws	-0.28		Crippen Method
logp	-0.979		Crippen Method
mcvol	71.050	ml/mol	McGowan Method

## Sources

<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=C16681702&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C16681702&amp;Units=SI</a>
<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>

## Legend

<b>chs:</b>	Standard solid enthalpy of combustion
<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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