

# Acetic acid, nitrilotri-

<b>Other names:</b>	nitrilotriacetic acid
<b>Inchi:</b>	InChI=1S/C6H9NO6/c8-4(9)1-7(2-5(10)11)3-6(12)13/h1-3H2,(H,8,9)(H,10,11)(H,12,13)
<b>InchiKey:</b>	MGFYIUFZLHCRTH-UHFFFAOYSA-N
<b>Formula:</b>	C6H9NO6
<b>SMILES:</b>	O=C(O)CN(CC(=O)O)CC(=O)O
<b>Mol. weight [g/mol]:</b>	191.14
<b>CAS:</b>	139-13-9

## Physical Properties

Property code	Value	Unit	Source
gf	-686.80	kJ/mol	Joback Method
hf	-894.07	kJ/mol	Joback Method
hfs	-1311.90 ± 1.10	kJ/mol	NIST Webbook
hfus	31.38	kJ/mol	Joback Method
hvap	101.27	kJ/mol	Joback Method
log10ws	1.80		Crippen Method
logp	-1.458		Crippen Method
mcvol	127.700	ml/mol	McGowan Method
pc	5644.74	kPa	Joback Method
tb	787.27	K	Joback Method
tc	970.10	K	Joback Method
tf	522.10	K	Joback Method
vc	0.465	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	357.78	J/mol×K	787.27	Joback Method
cpg	363.45	J/mol×K	817.74	Joback Method
cpg	368.74	J/mol×K	848.21	Joback Method
cpg	373.66	J/mol×K	878.68	Joback Method
cpg	378.23	J/mol×K	909.16	Joback Method
cpg	382.47	J/mol×K	939.63	Joback Method
cpg	386.40	J/mol×K	970.10	Joback 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=C139139&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C139139&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfs:</b>	Solid phase enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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