

# Cyclopentane, (nitromethylene)-

<b>Inchi:</b>	InChI=1S/C6H9NO2/c8-7(9)5-6-3-1-2-4-6/h5H,1-4H2
<b>InchiKey:</b>	FCFLHKHBKPPQQY-UHFFFAOYSA-N
<b>Formula:</b>	C6H9NO2
<b>SMILES:</b>	O=[N+](O-)C=C1CCCC1
<b>Mol. weight [g/mol]:</b>	127.14
<b>CAS:</b>	27861-40-1

## Physical Properties

Property code	Value	Unit	Source
gf	124.91	kJ/mol	Joback Method
hf	-21.08	kJ/mol	Joback Method
hfus	15.84	kJ/mol	Joback Method
hvap	46.89	kJ/mol	Joback Method
log10ws	-2.66		Crippen Method
logp	1.721		Crippen Method
mcvol	97.660	ml/mol	McGowan Method
pc	4216.56	kPa	Joback Method
tb	515.11	K	Joback Method
tc	758.94	K	Joback Method
tf	326.49	K	Joback Method
vc	0.379	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.99	J/molxK	515.11	Joback Method
cpg	227.66	J/molxK	555.75	Joback Method
cpg	239.39	J/molxK	596.39	Joback Method
cpg	250.23	J/molxK	637.03	Joback Method
cpg	260.26	J/molxK	677.67	Joback Method
cpg	269.53	J/molxK	718.30	Joback Method
cpg	278.10	J/molxK	758.94	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=C27861401&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C27861401&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>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>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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