

# 1-(Nitromethyl)cyclohexene

<b>Inchi:</b>	InChI=1S/C7H11NO2/c9-8(10)6-7-4-2-1-3-5-7/h4H,1-3,5-6H2
<b>InchiKey:</b>	KEELANLBFIOZSH-UHFFFAOYSA-N
<b>Formula:</b>	C7H11NO2
<b>SMILES:</b>	O=[N+](O-)CC1=CCCCC1
<b>Mol. weight [g/mol]:</b>	141.17
<b>CAS:</b>	5330-61-0

## Physical Properties

Property code	Value	Unit	Source
gf	96.10	kJ/mol	Joback Method
hf	-77.60	kJ/mol	Joback Method
hfus	16.84	kJ/mol	Joback Method
hvap	49.46	kJ/mol	Joback Method
log10ws	-2.59		Crippen Method
logp	1.764		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3815.10	kPa	Joback Method
tb	539.76	K	Joback Method
tc	783.31	K	Joback Method
tf	337.16	K	Joback Method
vc	0.429	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.83	J/molxK	539.76	Joback Method
cpg	273.15	J/molxK	580.35	Joback Method
cpg	286.47	J/molxK	620.94	Joback Method
cpg	298.84	J/molxK	661.54	Joback Method
cpg	310.30	J/molxK	702.13	Joback Method
cpg	320.90	J/molxK	742.72	Joback Method
cpg	330.67	J/molxK	783.31	Joback 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>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=C5330610&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5330610&amp;Units=SI</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>mccvol:</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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