

# N-methylglucosamine

<b>Inchi:</b>	InChI=1S/C7H15NO5/c1-8-4(2-9)6(12)7(13)5(11)3-10/h2,4-8,10-13H,3H2,1H3
<b>InchiKey:</b>	LDDMACCNBZAMSG-UHFFFAOYSA-N
<b>Formula:</b>	C7H15NO5
<b>SMILES:</b>	CNC(C=O)C(O)C(O)C(O)CO
<b>Mol. weight [g/mol]:</b>	193.20
<b>CAS:</b>	3329-30-4

## Physical Properties

Property code	Value	Unit	Source
gf	-559.11	kJ/mol	Joback Method
hf	-849.96	kJ/mol	Joback Method
hfus	23.53	kJ/mol	Joback Method
hvap	109.50	kJ/mol	Joback Method
log10ws	1.28		Crippen Method
logp	-3.152		Crippen Method
mvol	144.520	ml/mol	McGowan Method
pc	5080.25	kPa	Joback Method
tb	825.35	K	Joback Method
tc	1010.96	K	Joback Method
tf	446.59	K	Joback Method
vc	0.531	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	449.83	J/molxK	825.35	Joback Method
cpg	457.02	J/molxK	856.28	Joback Method
cpg	463.77	J/molxK	887.22	Joback Method
cpg	470.10	J/molxK	918.15	Joback Method
cpg	476.03	J/molxK	949.09	Joback Method
cpg	481.58	J/molxK	980.02	Joback Method
cpg	486.77	J/molxK	1010.96	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=C3329304&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3329304&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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