

# L-Threonine, N-glycyl-

<b>Other names:</b>	N-glycyl-L-threonine
<b>Inchi:</b>	InChI=1S/C6H12N2O4/c1-3(9)5(6(11)12)8-4(10)2-7/h3,5,9H,2,7H2,1H3,(H,8,10)(H,11,12)
<b>InchiKey:</b>	OLIFSFOFKGKIRH-WVZVXSGGSA-N
<b>Formula:</b>	C6H12N2O4
<b>SMILES:</b>	CC(O)C(NC(=O)CN)C(=O)O
<b>Mol. weight [g/mol]:</b>	176.17
<b>CAS:</b>	7093-70-1

## Physical Properties

Property code	Value	Unit	Source
gf	-380.88	kJ/mol	Joback Method
hf	-620.09	kJ/mol	Joback Method
hfus	25.92	kJ/mol	Joback Method
hvap	92.10	kJ/mol	Joback Method
log10ws	0.68		Crippen Method
logp	-2.105		Crippen Method
mcvol	130.240	ml/mol	McGowan Method
pc	5116.65	kPa	Joback Method
tb	750.60	K	Joback Method
tc	941.11	K	Joback Method
tf	484.80	K	Joback Method
vc	0.473	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	372.55	J/molxK	750.60	Joback Method
cpg	379.85	J/molxK	782.35	Joback Method
cpg	386.69	J/molxK	814.10	Joback Method
cpg	393.08	J/molxK	845.86	Joback Method
cpg	399.03	J/molxK	877.61	Joback Method
cpg	404.56	J/molxK	909.36	Joback Method
cpg	409.69	J/molxK	941.11	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C7093701&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7093701&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>
<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>

# 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>hvp:</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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