

# L-Alanine, N-acetyl-, methyl ester

<b>Inchi:</b>	InChI=1S/C6H11NO3/c1-4(6(9)10-3)7-5(2)8/h4H,1-3H3,(H,7,8)/t4-/m1/s1
<b>InchiKey:</b>	FQGVVDYNRHNTCK-SCSAIBSYSA-N
<b>Formula:</b>	C6H11NO3
<b>SMILES:</b>	COC(=O)C(C)NC(C)=O
<b>Mol. weight [g/mol]:</b>	145.16
<b>CAS:</b>	3619-02-1

## Physical Properties

Property code	Value	Unit	Source
gf	-276.25	kJ/mol	Joback Method
hf	-476.36	kJ/mol	Joback Method
hfus	17.26	kJ/mol	Joback Method
hvap	50.90	kJ/mol	Joback Method
log10ws	-0.27		Crippen Method
logp	-0.316		Crippen Method
mcvol	114.390	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	516.57	K	Joback Method
tc	711.62	K	Joback Method
tf	317.13	K	Joback Method
vc	0.430	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	256.69	J/molxK	516.57	Joback Method
cpg	266.93	J/molxK	549.08	Joback Method
cpg	276.73	J/molxK	581.59	Joback Method
cpg	286.08	J/molxK	614.10	Joback Method
cpg	294.98	J/molxK	646.61	Joback Method
cpg	303.44	J/molxK	679.11	Joback Method
cpg	311.45	J/molxK	711.62	Joback Method

# Sources

<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=C3619021&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3619021&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>

# 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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