

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

<b>Inchi:</b>	InChI=1S/C12H23NO3/c1-4-5-6-7-8-9-11(14)13-10(2)12(15)16-3/h10H,4-9H2,1-3H3,(H,1
<b>InchiKey:</b>	QTGVLHBHHGTRST-UHFFFAOYSA-N
<b>Formula:</b>	C12H23NO3
<b>SMILES:</b>	CCCCCCCC(=O)NC(C)C(=O)OC
<b>Mol. weight [g/mol]:</b>	229.32

## Physical Properties

Property code	Value	Unit	Source
gf	-225.73	kJ/mol	Joback Method
hf	-600.20	kJ/mol	Joback Method
hfus	32.80	kJ/mol	Joback Method
hvap	64.26	kJ/mol	Joback Method
log10ws	-2.78		Crippen Method
logp	2.025		Crippen Method
mcvol	198.930	ml/mol	McGowan Method
pc	1992.98	kPa	Joback Method
rinsol	1648.00		NIST Webbook
tb	653.85	K	Joback Method
tc	836.74	K	Joback Method
tf	384.75	K	Joback Method
vc	0.766	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	544.56	J/mol×K	653.85	Joback Method
cpg	559.39	J/mol×K	684.33	Joback Method
cpg	573.50	J/mol×K	714.81	Joback Method
cpg	586.89	J/mol×K	745.30	Joback Method
cpg	599.58	J/mol×K	775.78	Joback Method
cpg	611.57	J/mol×K	806.26	Joback Method
cpg	622.88	J/mol×K	836.74	Joback Method

# Sources

<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=U299722&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299722&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<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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