

# «beta»-Alanine, N-capryloyl-, propyl ester

<b>Inchi:</b>	InChI=1S/C14H27NO3/c1-3-5-6-7-8-9-13(16)15-11-10-14(17)18-12-4-2/h3-12H2,1-2H3,(
<b>InchiKey:</b>	NWDIUUYIHVIOJD-UHFFFAOYSA-N
<b>Formula:</b>	C14H27NO3
<b>SMILES:</b>	CCCCCCCC(=O)NCCC(=O)OCCC
<b>Mol. weight [g/mol]:</b>	257.37

## Physical Properties

Property code	Value	Unit	Source
gf	-206.45	kJ/mol	Joback Method
hf	-636.20	kJ/mol	Joback Method
hfus	41.50	kJ/mol	Joback Method
hvap	69.10	kJ/mol	Joback Method
log10ws	-3.51		Crippen Method
logp	2.806		Crippen Method
mcvol	227.110	ml/mol	McGowan Method
pc	1679.66	kPa	Joback Method
rinsol	1983.00		NIST Webbook
tb	700.05	K	Joback Method
tc	879.07	K	Joback Method
tf	422.29	K	Joback Method
vc	0.884	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	652.07	J/mol×K	700.05	Joback Method
cpg	667.62	J/mol×K	729.89	Joback Method
cpg	682.40	J/mol×K	759.72	Joback Method
cpg	696.42	J/mol×K	789.56	Joback Method
cpg	709.69	J/mol×K	819.39	Joback Method
cpg	722.24	J/mol×K	849.23	Joback Method
cpg	734.07	J/mol×K	879.07	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=U321807&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321807&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>

# 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>rinpola:</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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