

# DL-Alanine, N-methyl-N-(3-chloro-2-methylpropoxycarbonyl)-, octyl ester

InChI: InChI=1S/C17H32ClNO4/c1-5-6-7-8-9-10-11-22-16(20)15(3)19(4)17(21)23-13-14(2)12-1  
InChIKey: BVZRUGBSEAIIBC-UHFFFAOYSA-N

Formula: C17H32ClNO4

SMILES: CCCCCCOC(=O)C(C)N(C)C(=O)OCC(C)CCl

Mol. weight [g/mol]: 349.89

## Physical Properties

Property code	Value	Unit	Source
gf	-281.61	kJ/mol	Joback Method
hf	-842.58	kJ/mol	Joback Method
hfus	45.53	kJ/mol	Joback Method
hvap	77.40	kJ/mol	Joback Method
log10ws	-4.23		Crippen Method
logp	4.222		Crippen Method
mcvol	287.490	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	789.93	K	Joback Method
tc	975.97	K	Joback Method
tf	458.06	K	Joback Method
vc	1.091	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.58	J/mol×K	789.93	Joback Method
cpg	882.09	J/mol×K	820.94	Joback Method
cpg	897.62	J/mol×K	851.94	Joback Method
cpg	912.19	J/mol×K	882.95	Joback Method
cpg	925.81	J/mol×K	913.96	Joback Method
cpg	938.49	J/mol×K	944.97	Joback Method
cpg	950.27	J/mol×K	975.97	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U392770&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392770&amp;Units=SI</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>rinp:</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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