

# DL-Alanine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, hexadecyl ester

InChI: InChI=1S/C29H57NO4/c1-6-9-11-12-13-14-15-16-17-18-19-20-21-22-24-33-28(31)26(4)  
InChIKey: MGGYQPOJQUQFKP-UHFFFAOYSA-N

Formula: C29H57NO4

SMILES: CCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 483.77

## Physical Properties

Property code	Value	Unit	Source
gf	-168.64	kJ/mol	Joback Method
hf	-1074.52	kJ/mol	Joback Method
hfus	72.41	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Joback Method
log10ws	-9.10		Crippen Method
logp	8.684		Crippen Method
mvol	444.330	ml/mol	McGowan Method
pc	658.81	kPa	Joback Method
rinpol	3074.00		NIST Webbook
rinpol	3074.00		NIST Webbook
tb	1027.06	K	Joback Method
tc	1282.05	K	Joback Method
tf	563.38	K	Joback Method
vc	1.714	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.71	J/molxK	1027.06	Joback Method
cpg	1609.03	J/molxK	1069.56	Joback Method
cpg	1630.06	J/molxK	1112.06	Joback Method
cpg	1648.91	J/molxK	1154.56	Joback Method
cpg	1665.69	J/molxK	1197.05	Joback Method
cpg	1680.51	J/molxK	1239.55	Joback Method
cpg	1693.49	J/molxK	1282.05	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=U392667&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392667&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>h vap:</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>r in pol:</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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