

# DL-Alanine, N-methyl-N-(but-4-en-1-yloxy-carbonyl)-, tetradecyl ester

InChI: CN(C)C(=O)OCCCCCCCCCCCCCCC  
InChIKey: MYMNEGYESZVIGQ-UHFFFAOYSA-N

Formula: C<sub>23</sub>H<sub>43</sub>NO<sub>4</sub>

SMILES: C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 397.59

## Physical Properties

Property code	Value	Unit	Source
gf	-128.88	kJ/mol	Joback Method
hf	-819.97	kJ/mol	Joback Method
hfus	59.12	kJ/mol	Joback Method
hvap	86.09	kJ/mol	Joback Method
log10ws	-6.69		Crippen Method
logp	6.264		Crippen Method
mvol	355.490	ml/mol	McGowan Method
pc	926.11	kPa	Joback Method
rinpol	2590.00		NIST Webbook
rinpol	2590.00		NIST Webbook
tb	886.90	K	Joback Method
tc	1085.96	K	Joback Method
tf	509.00	K	Joback Method
vc	1.365	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.66	J/mol×K	886.90	Joback Method
cpg	1189.89	J/mol×K	920.08	Joback Method
cpg	1207.84	J/mol×K	953.25	Joback Method
cpg	1224.53	J/mol×K	986.43	Joback Method
cpg	1240.03	J/mol×K	1019.61	Joback Method
cpg	1254.36	J/mol×K	1052.78	Joback Method
cpg	1267.57	J/mol×K	1085.96	Joback Method

# Sources

<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=U392739&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392739&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.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>

# 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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