

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

InChI: InChI=1S/C24H45NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-21-28-23(26)22(3)25(4)  
InChIKey: SXSFKZDZBESHM-UHFFFAOYSA-N

Formula: C<sub>24</sub>H<sub>45</sub>NO<sub>4</sub>

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

Mol. weight [g/mol]: 411.62

## Physical Properties

Property code	Value	Unit	Source
gf	-120.46	kJ/mol	Joback Method
hf	-840.61	kJ/mol	Joback Method
hfus	61.71	kJ/mol	Joback Method
hvap	88.31	kJ/mol	Joback Method
log10ws	-7.11		Crippen Method
logp	6.654		Crippen Method
mvol	369.580	ml/mol	McGowan Method
pc	874.28	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	909.78	K	Joback Method
tc	1115.00	K	Joback Method
tf	520.27	K	Joback Method
vc	1.421	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1233.52	J/mol×K	909.78	Joback Method
cpg	1253.25	J/mol×K	943.98	Joback Method
cpg	1271.60	J/mol×K	978.19	Joback Method
cpg	1288.62	J/mol×K	1012.39	Joback Method
cpg	1304.34	J/mol×K	1046.59	Joback Method
cpg	1318.83	J/mol×K	1080.79	Joback Method
cpg	1332.12	J/mol×K	1115.00	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=U392740&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392740&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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