

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

InChI: InChI=1S/C20H37NO4/c1-5-7-9-10-11-12-13-14-15-17-24-19(22)18(3)21(4)20(23)25-16-17  
InChIKey: JCAZCXJQNUQAAT-UHFFFAOYSA-N

Formula: C20H37NO4

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

Mol. weight [g/mol]: 355.51

## Physical Properties

Property code	Value	Unit	Source
gf	-154.14	kJ/mol	Joback Method
hf	-758.05	kJ/mol	Joback Method
hfus	51.35	kJ/mol	Joback Method
hvap	79.41	kJ/mol	Joback Method
log10ws	-5.43		Crippen Method
logp	5.093		Crippen Method
mvol	313.220	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
rinpol	2298.00		NIST Webbook
rinpol	2298.00		NIST Webbook
tb	818.26	K	Joback Method
tc	1004.42	K	Joback Method
tf	475.19	K	Joback Method
vc	1.196	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	985.84	J/molxK	818.26	Joback Method
cpg	1003.77	J/molxK	849.29	Joback Method
cpg	1020.64	J/molxK	880.31	Joback Method
cpg	1036.47	J/molxK	911.34	Joback Method
cpg	1051.29	J/molxK	942.36	Joback Method
cpg	1065.13	J/molxK	973.39	Joback Method
cpg	1078.02	J/molxK	1004.42	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=U392736&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392736&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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