

# DL-Alanine, N-methyl-N-(but-2-yn-1-yloxy carbonyl)-, dodecyl ester

InChI: InChI=1S/C21H37NO4/c1-5-7-9-10-11-12-13-14-15-16-18-25-20(23)19(3)22(4)21(24)26-2  
InChIKey: RXLRHOQCBJYZDP-UHFFFAOYSA-N

Formula: C21H37NO4  
SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCC  
Mol. weight [g/mol]: 367.52

## Physical Properties

Property code	Value	Unit	Source
gf	-30.76	kJ/mol	Joback Method
hf	-631.82	kJ/mol	Joback Method
hfus	58.34	kJ/mol	Joback Method
hvap	84.46	kJ/mol	Joback Method
log10ws	-5.79		Crippen Method
logp	4.931		Crippen Method
mvol	323.010	ml/mol	McGowan Method
pc	1129.10	kPa	Joback Method
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	853.46	K	Joback Method
tc	1048.40	K	Joback Method
tf	594.32	K	Joback Method
vc	1.234	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1023.74	J/molxK	853.46	Joback Method
cpg	1041.57	J/molxK	885.95	Joback Method
cpg	1058.25	J/molxK	918.44	Joback Method
cpg	1073.81	J/molxK	950.93	Joback Method
cpg	1088.26	J/molxK	983.42	Joback Method
cpg	1101.64	J/molxK	1015.91	Joback Method
cpg	1113.97	J/molxK	1048.40	Joback Method

# Sources

<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=U392724&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392724&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>

# 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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