

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

InChI: InChI=1S/C25H45NO4/c1-5-7-9-10-11-12-13-14-15-16-17-18-19-20-22-29-24(27)23(3)26  
InChIKey: RIUZWFKSRNAUQJ-UHFFFAOYSA-N

Formula: C25H45NO4

SMILES: CC#CCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCCCCCC

Mol. weight [g/mol]: 423.63

## Physical Properties

Property code	Value	Unit	Source
gf	2.92	kJ/mol	Joback Method
hf	-714.38	kJ/mol	Joback Method
hfus	68.70	kJ/mol	Joback Method
hvap	93.36	kJ/mol	Joback Method
log10ws	-7.47		Crippen Method
logp	6.491		Crippen Method
mvol	379.370	ml/mol	McGowan Method
pc	885.77	kPa	Joback Method
rinpol	2878.00		NIST Webbook
rinpol	2878.00		NIST Webbook
tb	944.98	K	Joback Method
tc	1157.68	K	Joback Method
tf	639.40	K	Joback Method
vc	1.458	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1272.35	J/molxK	944.98	Joback Method
cpg	1291.60	J/molxK	980.43	Joback Method
cpg	1309.37	J/molxK	1015.88	Joback Method
cpg	1325.71	J/molxK	1051.33	Joback Method
cpg	1340.66	J/molxK	1086.78	Joback Method
cpg	1354.29	J/molxK	1122.23	Joback Method
cpg	1366.62	J/molxK	1157.68	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=U392727&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392727&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>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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