

# DL-Valine, N-methyl-N-(but-2-yn-1-yloxycarbonyl)-, tetradecyl ester

InChI: 1S/C25H45NO4/c1-6-8-10-11-12-13-14-15-16-17-18-19-21-29-24(27)23(22(3)4)20  
InChIKey: VIZSKYRDLIXXEH-UHFFFAOYSA-N

Formula: C25H45NO4  
SMILES: CC#CCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCCCC)C(C)C  
Mol. weight [g/mol]: 423.63

## Physical Properties

Property code	Value	Unit	Source
gf	0.48	kJ/mol	Joback Method
hf	-719.66	kJ/mol	Joback Method
hfus	65.18	kJ/mol	Joback Method
hvap	92.98	kJ/mol	Joback Method
log10ws	-7.23		Crippen Method
logp	6.347		Crippen Method
mcvol	379.370	ml/mol	McGowan Method
pc	890.00	kPa	Joback Method
rinpol	2840.00		NIST Webbook
rinpol	2840.00		NIST Webbook
tb	944.54	K	Joback Method
tc	1156.74	K	Joback Method
tf	624.40	K	Joback Method
vc	1.452	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1272.74	J/molxK	944.54	Joback Method
cpg	1291.90	J/molxK	979.91	Joback Method
cpg	1309.58	J/molxK	1015.27	Joback Method
cpg	1325.83	J/molxK	1050.64	Joback Method
cpg	1340.68	J/molxK	1086.01	Joback Method
cpg	1354.20	J/molxK	1121.37	Joback Method
cpg	1366.42	J/molxK	1156.74	Joback Method

# Sources

<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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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=U392959&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392959&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>hvap:</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>rinpola:</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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