

# DL-Valine, N-methyl-N-(but-3-yn-1-yloxy carbonyl)-, tridecyl ester

InChI: InChI=1S/C24H43NO4/c1-6-8-10-11-12-13-14-15-16-17-18-20-28-23(26)22(21(3)4)25(5)  
InChIKey: UELGDAIDYYKXHT-UHFFFAOYSA-N

Formula: C24H43NO4

SMILES: C#CCCOC(=O)N(C)C(C(=O)OCCCCCCCCCCCCC)C(C)C

Mol. weight [g/mol]: 409.60

## Physical Properties

Property code	Value	Unit	Source
gf	12.33	kJ/mol	Joback Method
hf	-679.42	kJ/mol	Joback Method
hfus	62.44	kJ/mol	Joback Method
hvap	88.46	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.957		Crippen Method
mcvol	365.280	ml/mol	McGowan Method
pc	936.35	kPa	Joback Method
rinpol	2650.00		NIST Webbook
rinpol	2650.00		NIST Webbook
tb	902.78	K	Joback Method
tc	1105.26	K	Joback Method
tf	554.00	K	Joback Method
vc	1.395	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1202.75	J/mol×K	902.78	Joback Method
cpg	1221.74	J/mol×K	936.53	Joback Method
cpg	1239.43	J/mol×K	970.27	Joback Method
cpg	1255.87	J/mol×K	1004.02	Joback Method
cpg	1271.10	J/mol×K	1037.77	Joback Method
cpg	1285.16	J/mol×K	1071.52	Joback Method
cpg	1298.11	J/mol×K	1105.26	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=U392939&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392939&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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