

# DL-Valine, N-methyl-N-(vinylloxycarbonyl)-, undecyl ester

<b>Inchi:</b>	InChI=1S/C20H37NO4/c1-6-8-9-10-11-12-13-14-15-16-25-19(22)18(17(3)4)21(5)20(23)2
<b>InchiKey:</b>	YZXCLFBEGMRVOF-UHFFFAOYSA-N
<b>Formula:</b>	C20H37NO4
<b>SMILES:</b>	C=COC(=O)N(C)C(C(=O)OCCCCCCCCCCC)C(C)C
<b>Mol. weight [g/mol]:</b>	355.51

## Physical Properties

Property code	Value	Unit	Source
gf	-156.58	kJ/mol	Joback Method
hf	-763.33	kJ/mol	Joback Method
hfus	47.82	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-5.69		Crippen Method
logp	5.297		Crippen Method
mvol	313.220	ml/mol	McGowan Method
pc	1118.56	kPa	Joback Method
rinpol	2236.00		NIST Webbook
rinpol	2236.00		NIST Webbook
tb	817.82	K	Joback Method
tc	1004.78	K	Joback Method
tf	460.19	K	Joback Method
vc	1.190	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	986.33	J/mol×K	817.82	Joback Method
cpg	1004.33	J/mol×K	848.98	Joback Method
cpg	1021.26	J/mol×K	880.14	Joback Method
cpg	1037.13	J/mol×K	911.30	Joback Method
cpg	1051.97	J/mol×K	942.46	Joback Method
cpg	1065.82	J/mol×K	973.62	Joback Method
cpg	1078.69	J/mol×K	1004.78	Joback Method

# Sources

<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=U393042&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393042&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>

# 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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