

# DL-Alanine, N-methyl-N-(vinylloxycarbonyl)-, octyl ester

<b>Inchi:</b>	InChI=1S/C15H27NO4/c1-5-7-8-9-10-11-12-20-14(17)13(3)16(4)15(18)19-6-2/h6,13H,2,
<b>InchiKey:</b>	NNVWRHAWUBJHQM-UHFFFAOYSA-N
<b>Formula:</b>	C15H27NO4
<b>SMILES:</b>	C=COC(=O)N(C)C(C)C(=O)OCCCCCCCC
<b>Mol. weight [g/mol]:</b>	285.38

## Physical Properties

Property code	Value	Unit	Source
gf	-196.24	kJ/mol	Joback Method
hf	-654.85	kJ/mol	Joback Method
hfus	38.40	kJ/mol	Joback Method
hvap	68.28	kJ/mol	Joback Method
log10ws	-3.83		Crippen Method
logp	3.490		Crippen Method
mcvol	242.770	ml/mol	McGowan Method
pc	1577.21	kPa	Joback Method
rinpol	1843.00		NIST Webbook
rinpol	1843.00		NIST Webbook
tb	703.86	K	Joback Method
tc	883.16	K	Joback Method
tf	418.84	K	Joback Method
vc	0.916	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	694.30	J/mol×K	703.86	Joback Method
cpg	710.33	J/mol×K	733.74	Joback Method
cpg	725.54	J/mol×K	763.63	Joback Method
cpg	739.92	J/mol×K	793.51	Joback Method
cpg	753.51	J/mol×K	823.39	Joback Method
cpg	766.31	J/mol×K	853.27	Joback Method
cpg	778.35	J/mol×K	883.16	Joback Method

# Sources

<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=U392754&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392754&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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