

# DL-Alanine, N-methyl-N-(but-4-en-1-yloxy carbonyl)-, but-4-en-1-yl ester

InChI: CN(C)C(=O)OCC=C  
InChIKey: GLVVDXACJLNFQD-UHFFFAOYSA-N

Formula: C<sub>13</sub>H<sub>21</sub>NO<sub>4</sub>

SMILES: C=CCCOC(=O)C(C)N(C)C(=O)OCCC=C

Mol. weight [g/mol]: 255.31

## Physical Properties

Property code	Value	Unit	Source
gf	-125.24	kJ/mol	Joback Method
hf	-488.14	kJ/mol	Joback Method
hfus	31.94	kJ/mol	Joback Method
hvap	63.16	kJ/mol	Joback Method
log10ws	-2.36		Crippen Method
logp	2.139		Crippen Method
mcvol	210.290	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
tb	654.78	K	Joback Method
tc	837.65	K	Joback Method
tf	394.54	K	Joback Method
vc	0.785	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	562.47	J/mol×K	654.78	Joback Method
cpg	577.08	J/mol×K	685.26	Joback Method
cpg	590.94	J/mol×K	715.74	Joback Method
cpg	604.06	J/mol×K	746.21	Joback Method
cpg	616.45	J/mol×K	776.69	Joback Method
cpg	628.14	J/mol×K	807.17	Joback Method
cpg	639.13	J/mol×K	837.65	Joback Method

# Sources

<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=U392744&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392744&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>

# 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>rlnpol:</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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