

# DL-Alanyl-DL-alanine, N,N'-dimethyl-N'-(but-4-en-1-yloxycarbonyl)-, hexyl ester

InChI: InChI=1S/C19H34N2O5/c1-7-9-11-12-14-25-18(23)16(4)20(5)17(22)15(3)21(6)19(24)26-  
InChIKey: CNQDNEOADCGHDK-UHFFFAOYSA-N

Formula: C19H34N2O5

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

Mol. weight [g/mol]: 370.48

## Physical Properties

Property code	Value	Unit	Source
gf	-183.14	kJ/mol	Joback Method
hf	-787.74	kJ/mol	Joback Method
hfus	49.85	kJ/mol	Joback Method
hvap	85.59	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.990		Crippen Method
mcvol	310.680	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
tb	861.25	K	Joback Method
tc	1056.62	K	Joback Method
tf	531.32	K	Joback Method
vc	1.159	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	990.71	J/mol×K	861.25	Joback Method
cpg	1006.95	J/mol×K	893.81	Joback Method
cpg	1022.05	J/mol×K	926.37	Joback Method
cpg	1036.07	J/mol×K	958.93	Joback Method
cpg	1049.02	J/mol×K	991.50	Joback Method
cpg	1060.96	J/mol×K	1024.06	Joback Method
cpg	1071.90	J/mol×K	1056.62	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392746&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392746&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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>h vap:</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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