

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

InChI: InChI=1S/C18H32N2O5/c1-7-9-11-13-24-17(22)15(4)19(5)16(21)14(3)20(6)18(23)25-12-2  
InChIKey: BGLZMIMFUVBQD-UHFFFAOYSA-N

Formula: C18H32N2O5

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

Mol. weight [g/mol]: 356.46

## Physical Properties

Property code	Value	Unit	Source
gf	-191.56	kJ/mol	Joback Method
hf	-767.10	kJ/mol	Joback Method
hfus	47.26	kJ/mol	Joback Method
hvap	83.36	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.600		Crippen Method
mcvol	296.590	ml/mol	McGowan Method
pc	1334.91	kPa	Joback Method
rinpol	2214.00		NIST Webbook
rinpol	2214.00		NIST Webbook
tb	838.37	K	Joback Method
tc	1030.97	K	Joback Method
tf	520.05	K	Joback Method
vc	1.103	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	931.10	J/molxK	838.37	Joback Method
cpg	947.01	J/molxK	870.47	Joback Method
cpg	961.85	J/molxK	902.57	Joback Method
cpg	975.65	J/molxK	934.67	Joback Method
cpg	988.44	J/molxK	966.77	Joback Method
cpg	1000.25	J/molxK	998.87	Joback Method
cpg	1011.11	J/molxK	1030.97	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=U392745&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392745&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>

# 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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