

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

InChI: InChI=1S/C21H38N2O5/c1-7-9-11-12-13-14-16-27-20(25)18(4)22(5)19(24)17(3)23(6)21

InChIKey: VGHUQSGXPYHHDH-UHFFFAOYSA-N

Formula: C21H38N2O5

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

Mol. weight [g/mol]: 398.54

## Physical Properties

Property code	Value	Unit	Source
gf	-166.30	kJ/mol	Joback Method
hf	-829.02	kJ/mol	Joback Method
hfus	55.03	kJ/mol	Joback Method
hvap	90.04	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.770		Crippen Method
mvol	338.860	ml/mol	McGowan Method
pc	1092.82	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	907.01	K	Joback Method
tc	1110.45	K	Joback Method
tf	553.86	K	Joback Method
vc	1.270	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1111.97	J/molxK	907.01	Joback Method
cpg	1128.90	J/molxK	940.92	Joback Method
cpg	1144.57	J/molxK	974.82	Joback Method
cpg	1159.03	J/molxK	1008.73	Joback Method
cpg	1172.30	J/molxK	1042.64	Joback Method
cpg	1184.45	J/molxK	1076.54	Joback Method
cpg	1195.52	J/molxK	1110.45	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392748&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392748&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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>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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