

# DL-Alanine, N-methyl-N-(2-benzyloxyethoxycarbonyl)-, heptyl ester

InChI: InChI=1S/C21H33NO5/c1-4-5-6-7-11-14-26-20(23)18(2)22(3)21(24)27-16-15-25-17-19-1  
InChIKey: CKCABGZBAOYKBV-UHFFFAOYSA-N

Formula: C21H33NO5

SMILES: CCCCCCOC(=O)C(C)N(C)C(=O)OCCOCc1ccccc1

Mol. weight [g/mol]: 379.49

## Physical Properties

Property code	Value	Unit	Source
gf	-226.15	kJ/mol	Joback Method
hf	-799.81	kJ/mol	Joback Method
hfus	50.45	kJ/mol	Joback Method
hvap	86.99	kJ/mol	Joback Method
log10ws	-4.68		Crippen Method
logp	4.174		Crippen Method
mcvol	313.720	ml/mol	McGowan Method
pc	1255.70	kPa	Joback Method
rinpol	2594.00		NIST Webbook
rinpol	2594.00		NIST Webbook
tb	893.56	K	Joback Method
tc	1098.05	K	Joback Method
tf	536.87	K	Joback Method
vc	1.181	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1010.72	J/molxK	893.56	Joback Method
cpg	1026.71	J/molxK	927.64	Joback Method
cpg	1041.37	J/molxK	961.72	Joback Method
cpg	1054.76	J/molxK	995.80	Joback Method
cpg	1066.89	J/molxK	1029.89	Joback Method
cpg	1077.79	J/molxK	1063.97	Joback Method
cpg	1087.49	J/molxK	1098.05	Joback Method

# Sources

<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.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>
<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=U392691&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392691&amp;Units=SI</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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