

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

InChI: InChI=1S/C26H43NO5/c1-4-5-6-7-8-9-10-11-12-16-19-31-25(28)23(2)27(3)26(29)32-21-3  
InChIKey: PHDNOHHGDOQAPJ-UHFFFAOYSA-N

Formula: C26H43NO5

SMILES: CCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCOCc1cccc1

Mol. weight [g/mol]: 449.62

## Physical Properties

Property code	Value	Unit	Source
gf	-184.05	kJ/mol	Joback Method
hf	-903.01	kJ/mol	Joback Method
hfus	63.40	kJ/mol	Joback Method
hvap	98.12	kJ/mol	Joback Method
log10ws	-6.78		Crippen Method
logp	6.124		Crippen Method
mvol	384.170	ml/mol	McGowan Method
pc	917.16	kPa	Joback Method
rinpol	3082.00		NIST Webbook
rinpol	3082.00		NIST Webbook
tb	1007.96	K	Joback Method
tc	1236.38	K	Joback Method
tf	593.22	K	Joback Method
vc	1.462	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1318.05	J/mol×K	1007.96	Joback Method
cpg	1335.00	J/mol×K	1046.03	Joback Method
cpg	1350.20	J/mol×K	1084.10	Joback Method
cpg	1363.69	J/mol×K	1122.17	Joback Method
cpg	1375.53	J/mol×K	1160.24	Joback Method
cpg	1385.79	J/mol×K	1198.31	Joback Method
cpg	1394.52	J/mol×K	1236.38	Joback Method

# Sources

<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=U392696&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392696&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r in pol:</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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