

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

InChI: InChI=1S/C27H45NO5/c1-4-5-6-7-8-9-10-11-12-13-17-20-32-26(29)24(2)28(3)27(30)33-34  
InChIKey: OJZZVKJDHYTLQJ-UHFFFAOYSA-N

Formula: C27H45NO5

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

Mol. weight [g/mol]: 463.65

## Physical Properties

Property code	Value	Unit	Source
gf	-175.63	kJ/mol	Joback Method
hf	-923.65	kJ/mol	Joback Method
hfus	65.99	kJ/mol	Joback Method
hvap	100.35	kJ/mol	Joback Method
log10ws	-7.19		Crippen Method
logp	6.514		Crippen Method
mvol	398.260	ml/mol	McGowan Method
pc	866.07	kPa	Joback Method
rinpol	3184.00		NIST Webbook
rinpol	3184.00		NIST Webbook
tb	1030.84	K	Joback Method
tc	1267.31	K	Joback Method
tf	604.49	K	Joback Method
vc	1.518	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1380.70	J/molxK	1030.84	Joback Method
cpg	1397.91	J/molxK	1070.25	Joback Method
cpg	1413.22	J/molxK	1109.66	Joback Method
cpg	1426.70	J/molxK	1149.08	Joback Method
cpg	1438.43	J/molxK	1188.49	Joback Method
cpg	1448.46	J/molxK	1227.90	Joback Method
cpg	1456.87	J/molxK	1267.31	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=U392697&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392697&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>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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