

# DL-Alanine, N-methyl-N-hexyloxycarbonyl-, hexadecyl ester

<b>Inchi:</b>	InChI=1S/C27H53NO4/c1-5-7-9-11-12-13-14-15-16-17-18-19-20-22-23-31-26(29)25(3)2
<b>InchiKey:</b>	JSBOFJBERUMZFT-UHFFFAOYSA-N
<b>Formula:</b>	C27H53NO4
<b>SMILES:</b>	CCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	455.71

## Physical Properties

Property code	Value	Unit	Source
gf	-183.04	kJ/mol	Joback Method
hf	-1027.96	kJ/mol	Joback Method
hfus	70.76	kJ/mol	Joback Method
hvap	95.66	kJ/mol	Joback Method
log10ws	-8.51		Crippen Method
logp	8.048		Crippen Method
mvol	416.150	ml/mol	McGowan Method
pc	725.75	kPa	Joback Method
rinpol	2962.00		NIST Webbook
rinpol	2962.00		NIST Webbook
tb	981.74	K	Joback Method
tc	1215.30	K	Joback Method
tf	555.84	K	Joback Method
vc	1.607	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1455.24	J/molxK	981.74	Joback Method
cpg	1477.43	J/molxK	1020.67	Joback Method
cpg	1497.70	J/molxK	1059.59	Joback Method
cpg	1516.15	J/molxK	1098.52	Joback Method
cpg	1532.85	J/molxK	1137.44	Joback Method
cpg	1547.86	J/molxK	1176.37	Joback Method
cpg	1561.28	J/molxK	1215.30	Joback Method

# Sources

<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=U392645&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392645&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>

# 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>hvap:</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>rlnpol:</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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