

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

InChI: InChI=1S/C25H49NO4/c1-6-9-11-12-13-14-15-16-17-18-20-29-24(27)22(4)26(5)25(28)3  
InChIKey: GVANWNOWQOTEGZ-UHFFFAOYSA-N

Formula: C25H49NO4

SMILES: CCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCC(CC)CCCC

Mol. weight [g/mol]: 427.66

## Physical Properties

Property code	Value	Unit	Source
gf	-202.32	kJ/mol	Joback Method
hf	-991.96	kJ/mol	Joback Method
hfus	62.05	kJ/mol	Joback Method
hvap	90.82	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	7.124		Crippen Method
mvol	387.970	ml/mol	McGowan Method
pc	810.76	kPa	Joback Method
rinpol	2686.00		NIST Webbook
rinpol	2686.00		NIST Webbook
tb	935.54	K	Joback Method
tc	1148.84	K	Joback Method
tf	518.30	K	Joback Method
vc	1.490	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1326.77	J/molxK	935.54	Joback Method
cpg	1347.53	J/molxK	971.09	Joback Method
cpg	1366.71	J/molxK	1006.64	Joback Method
cpg	1384.35	J/molxK	1042.19	Joback Method
cpg	1400.51	J/molxK	1077.74	Joback Method
cpg	1415.24	J/molxK	1113.29	Joback Method
cpg	1428.60	J/molxK	1148.84	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.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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U392663&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392663&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>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>rinpola:</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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