

# DL-Alanine, N-methyl-N-decyloxycarbonyl-, tetradecyl ester

<b>Inchi:</b>	InChI=1S/C29H57NO4/c1-5-7-9-11-13-15-16-17-18-20-21-23-25-33-28(31)27(3)30(4)29
<b>InchiKey:</b>	GNXVJNDMGVFWLM-UHFFFAOYSA-N
<b>Formula:</b>	C29H57NO4
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCCCCC
<b>Mol. weight [g/mol]:</b>	483.77

## Physical Properties

Property code	Value	Unit	Source
gf	-166.20	kJ/mol	Joback Method
hf	-1069.24	kJ/mol	Joback Method
hfus	75.94	kJ/mol	Joback Method
hvap	100.12	kJ/mol	Joback Method
log10ws	-9.35		Crippen Method
logp	8.828		Crippen Method
mcvol	444.330	ml/mol	McGowan Method
pc	656.12	kPa	Joback Method
rinpol	3150.00		NIST Webbook
rinpol	3150.00		NIST Webbook
tb	1027.50	K	Joback Method
tc	1285.62	K	Joback Method
tf	578.38	K	Joback Method
vc	1.720	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1585.48	J/molxK	1027.50	Joback Method
cpg	1609.16	J/molxK	1070.52	Joback Method
cpg	1630.51	J/molxK	1113.54	Joback Method
cpg	1649.64	J/molxK	1156.56	Joback Method
cpg	1666.68	J/molxK	1199.58	Joback Method
cpg	1681.73	J/molxK	1242.60	Joback Method
cpg	1694.92	J/molxK	1285.62	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=U392684&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392684&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.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>

# 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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