

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

<b>Inchi:</b>	InChI=1S/C19H37NO4/c1-5-7-9-11-12-14-15-23-18(21)17(3)20(4)19(22)24-16-13-10-8-6
<b>InchiKey:</b>	JLWVQGJHFPISHH-UHFFFAOYSA-N
<b>Formula:</b>	C19H37NO4
<b>SMILES:</b>	CCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCC
<b>Mol. weight [g/mol]:</b>	343.50

## Physical Properties

Property code	Value	Unit	Source
gf	-250.40	kJ/mol	Joback Method
hf	-862.84	kJ/mol	Joback Method
hfus	50.04	kJ/mol	Joback Method
hvap	77.86	kJ/mol	Joback Method
log10ws	-5.16		Crippen Method
logp	4.927		Crippen Method
mvol	303.430	ml/mol	McGowan Method
pc	1153.78	kPa	Joback Method
rinpol	2221.00		NIST Webbook
rinpol	2221.00		NIST Webbook
tb	798.70	K	Joback Method
tc	981.66	K	Joback Method
tf	465.68	K	Joback Method
vc	1.159	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	952.38	J/mol×K	798.70	Joback Method
cpg	970.45	J/mol×K	829.19	Joback Method
cpg	987.50	J/mol×K	859.69	Joback Method
cpg	1003.53	J/mol×K	890.18	Joback Method
cpg	1018.56	J/mol×K	920.67	Joback Method
cpg	1032.62	J/mol×K	951.16	Joback Method
cpg	1045.73	J/mol×K	981.66	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=U392637&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392637&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>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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