

# DL-Alanine, N-methyl-N-((1R)-(-)-menthyloxycarbonyl)-, octadecyl ester

InChI: InChI=1S/C33H63NO4/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-25-37-32(35)  
InChIKey: NGPGFZRECDSDNR-UHFFFAOYSA-N

Formula: C33H63NO4

SMILES: CCCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OC1CC(C)CCC1C(C)C

Mol. weight [g/mol]: 537.86

## Physical Properties

Property code	Value	Unit	Source
gf	-125.93	kJ/mol	Joback Method
hf	-1143.44	kJ/mol	Joback Method
hfus	76.75	kJ/mol	Joback Method
hvap	108.44	kJ/mol	Joback Method
log10ws	-10.30		Crippen Method
logp	9.709		Crippen Method
mcvol	489.830	ml/mol	McGowan Method
pc	583.16	kPa	Joback Method
rinpol	3462.00		NIST Webbook
rinpol	3462.00		NIST Webbook
tb	1128.79	K	Joback Method
tc	1420.73	K	Joback Method
tf	607.36	K	Joback Method
vc	1.869	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1849.20	J/molxK	1128.79	Joback Method
cpg	1870.60	J/molxK	1177.45	Joback Method
cpg	1888.48	J/molxK	1226.10	Joback Method
cpg	1903.02	J/molxK	1274.76	Joback Method
cpg	1914.39	J/molxK	1323.41	Joback Method
cpg	1922.76	J/molxK	1372.07	Joback Method
cpg	1928.29	J/molxK	1420.73	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=U392805&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392805&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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