

# DL-Alanine, N-methyl-N-(3-chloropropoxycarbonyl)-, nonyl

Inchi:  
ester

InChI=1S/C17H32ClNO4/c1-4-5-6-7-8-9-10-13-22-16(20)15(2)19(3)17(21)23-14-11-12-1

InchiKey:

QQHCVZHBRUVFAB-UHFFFAOYSA-N

Formula:

C17H32ClNO4

SMILES:

CCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCI

Mol. weight [g/mol]:

349.89

## Physical Properties

Property code	Value	Unit	Source
gf	-279.17	kJ/mol	Joback Method
hf	-837.30	kJ/mol	Joback Method
hfus	49.05	kJ/mol	Joback Method
hvap	77.79	kJ/mol	Joback Method
log10ws	-4.48		Crippen Method
logp	4.366		Crippen Method
mcvol	287.490	ml/mol	McGowan Method
pc	1285.59	kPa	Joback Method
rinpol	2276.00		NIST Webbook
rinpol	2276.00		NIST Webbook
tb	790.37	K	Joback Method
tc	975.07	K	Joback Method
tf	473.06	K	Joback Method
vc	1.097	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	865.07	J/mol×K	790.37	Joback Method
cpg	881.46	J/mol×K	821.15	Joback Method
cpg	896.89	J/mol×K	851.94	Joback Method
cpg	911.38	J/mol×K	882.72	Joback Method
cpg	924.94	J/mol×K	913.50	Joback Method
cpg	937.59	J/mol×K	944.28	Joback Method
cpg	949.36	J/mol×K	975.07	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=U392781&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392781&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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