

# DL-Alanine, N-methyl-N-(3-chloropropoxycarbonyl)-, 3-chloropropyl ester

InChI: InChI=1S/C11H19Cl2NO4/c1-9(10(15)17-7-3-5-12)14(2)11(16)18-8-4-6-13/h9H,3-8H2,1-  
InChIKey: SJXUQVYJCJBCXSB-UHFFFAOYSA-N

Formula: C11H19Cl2NO4  
SMILES: CC(C(=O)OCCCCI)N(C)C(=O)OCCCCI  
Mol. weight [g/mol]: 300.18

## Physical Properties

Property code	Value	Unit	Source
gf	-341.62	kJ/mol	Joback Method
hf	-729.20	kJ/mol	Joback Method
hfus	37.71	kJ/mol	Joback Method
hvap	68.82	kJ/mol	Joback Method
log10ws	-2.12		Crippen Method
logp	2.244		Crippen Method
mcvol	215.190	ml/mol	McGowan Method
pc	1975.31	kPa	Joback Method
tb	690.52	K	Joback Method
tc	879.11	K	Joback Method
tf	435.36	K	Joback Method
vc	0.809	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	559.82	J/molxK	690.52	Joback Method
cpg	572.82	J/molxK	721.95	Joback Method
cpg	585.09	J/molxK	753.38	Joback Method
cpg	596.64	J/molxK	784.81	Joback Method
cpg	607.47	J/molxK	816.25	Joback Method
cpg	617.60	J/molxK	847.68	Joback Method
cpg	627.03	J/molxK	879.11	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=U392791&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U392791&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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

Latest version available from:

<https://www.chemeo.com/cid/93-333-9/DL-Alanine-N-methyl-N-3-chloropropoxycarbonyl-3-chloropropyl-ester.pdf>

Generated by Cheméo on 2024-04-19 22:40:23.619684737 +0000 UTC m=+15855672.540262052.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.