

# L-Alanine, N-(2-chlorobenzoyl)-, methyl ester

<b>Inchi:</b>	InChI=1S/C11H12ClNO3/c1-7(11(15)16-2)13-10(14)8-5-3-4-6-9(8)12/h3-7H,1-2H3,(H,13)
<b>InchiKey:</b>	IYECSEXZMPHUOA-UHFFFAOYSA-N
<b>Formula:</b>	C11H12ClNO3
<b>SMILES:</b>	COC(=O)C(C)NC(=O)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	241.67

## Physical Properties

Property code	Value	Unit	Source
gf	-143.30	kJ/mol	Joback Method
hf	-370.24	kJ/mol	Joback Method
hfus	28.06	kJ/mol	Joback Method
hvap	69.35	kJ/mol	Joback Method
log10ws	-2.73		Crippen Method
logp	1.631		Crippen Method
mcvol	173.320	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinsol	1772.00		NIST Webbook
tb	700.06	K	Joback Method
tc	924.27	K	Joback Method
tf	442.34	K	Joback Method
vc	0.651	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	435.75	J/mol×K	700.06	Joback Method
cpg	447.64	J/mol×K	737.43	Joback Method
cpg	458.64	J/mol×K	774.80	Joback Method
cpg	468.79	J/mol×K	812.17	Joback Method
cpg	478.10	J/mol×K	849.54	Joback Method
cpg	486.59	J/mol×K	886.90	Joback Method
cpg	494.28	J/mol×K	924.27	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=U299586&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U299586&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>r inpol:</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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