

# «beta»-Alanine, N-(2-chlorobenzoyl)-, undecyl ester

Inchi:	InChI=1S/C21H32ClNO3/c1-2-3-4-5-6-7-8-9-12-17-26-20(24)15-16-23-21(25)18-13-10-1
InchiKey:	OGLQUWIGLHDZMG-UHFFFAOYSA-N
Formula:	C21H32ClNO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccccc1Cl
Mol. weight [g/mol]:	381.94

## Physical Properties

Property code	Value	Unit	Source
gf	-56.66	kJ/mol	Joback Method
hf	-571.36	kJ/mol	Joback Method
hfus	57.48	kJ/mol	Joback Method
hvap	92.00	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.534		Crippen Method
mvol	314.220	ml/mol	McGowan Method
pc	1245.97	kPa	Joback Method
rinpol	3062.00		NIST Webbook
tb	929.30	K	Joback Method
tc	1140.86	K	Joback Method
tf	570.04	K	Joback Method
vc	1.218	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	994.05	J/mol×K	929.30	Joback Method
cpg	1009.00	J/mol×K	964.56	Joback Method
cpg	1022.80	J/mol×K	999.82	Joback Method
cpg	1035.50	J/mol×K	1035.08	Joback Method
cpg	1047.13	J/mol×K	1070.34	Joback Method
cpg	1057.75	J/mol×K	1105.60	Joback Method
cpg	1067.41	J/mol×K	1140.86	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=U321581&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321581&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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