

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

<b>Inchi:</b>	InChI=1S/C24H38ClNO3/c1-2-3-4-5-6-7-8-9-10-11-12-15-20-29-23(27)18-19-26-24(28)2
<b>InchiKey:</b>	WGPEOKJCBMIFIN-UHFFFAOYSA-N
<b>Formula:</b>	C24H38ClNO3
<b>SMILES:</b>	CCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	424.02

## Physical Properties

Property code	Value	Unit	Source
gf	-31.40	kJ/mol	Joback Method
hf	-633.28	kJ/mol	Joback Method
hfus	65.25	kJ/mol	Joback Method
hvap	98.68	kJ/mol	Joback Method
log10ws	-8.06		Crippen Method
logp	6.704		Crippen Method
mcvol	356.490	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
tb	997.94	K	Joback Method
tc	1221.89	K	Joback Method
tf	603.85	K	Joback Method
vc	1.385	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.73	J/molxK	997.94	Joback Method
cpg	1192.58	J/molxK	1035.26	Joback Method
cpg	1207.10	J/molxK	1072.59	Joback Method
cpg	1220.35	J/molxK	1109.91	Joback Method
cpg	1232.40	J/molxK	1147.24	Joback Method
cpg	1243.33	J/molxK	1184.56	Joback Method
cpg	1253.21	J/molxK	1221.89	Joback Method

# Sources

<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.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=U321583&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321583&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

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