

# «beta»-Alanine, N-(4-chlorobenzoyl)-, hexyl ester

Inchi:	InChI=1S/C16H22ClNO3/c1-2-3-4-5-12-21-15(19)10-11-18-16(20)13-6-8-14(17)9-7-13/h
InchiKey:	DOVGEOHEEVJQGX-UHFFFAOYSA-N
Formula:	C16H22ClNO3
SMILES:	CCCCCCOC(=O)CCNC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	311.80

## Physical Properties

Property code	Value	Unit	Source
gf	-98.76	kJ/mol	Joback Method
hf	-468.16	kJ/mol	Joback Method
hfus	44.53	kJ/mol	Joback Method
hvap	80.87	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	3.583		Crippen Method
mcvol	243.770	ml/mol	McGowan Method
pc	1806.16	kPa	Joback Method
rinpol	2493.00		NIST Webbook
rinpol	2493.00		NIST Webbook
tb	814.90	K	Joback Method
tc	1022.88	K	Joback Method
tf	513.69	K	Joback Method
vc	0.938	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	702.86	J/mol×K	814.90	Joback Method
cpg	716.54	J/mol×K	849.56	Joback Method
cpg	729.23	J/mol×K	884.23	Joback Method
cpg	740.98	J/mol×K	918.89	Joback Method
cpg	751.80	J/mol×K	953.55	Joback Method
cpg	761.74	J/mol×K	988.22	Joback Method
cpg	770.82	J/mol×K	1022.88	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=U321720&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321720&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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpola:</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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