

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

Inchi:	InChI=1S/C15H20ClNO3/c1-2-3-4-11-20-14(18)9-10-17-15(19)12-5-7-13(16)8-6-12/h5-8
InchiKey:	AEPLOPPDIMQBKI-UHFFFAOYSA-N
Formula:	C15H20ClNO3
SMILES:	CCCCCOC(=O)CCNC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	297.78

## Physical Properties

Property code	Value	Unit	Source
gf	-107.18	kJ/mol	Joback Method
hf	-447.52	kJ/mol	Joback Method
hfus	41.94	kJ/mol	Joback Method
hvap	78.65	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.193		Crippen Method
mcvol	229.680	ml/mol	McGowan Method
pc	1963.07	kPa	Joback Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook
tb	792.02	K	Joback Method
tc	1001.35	K	Joback Method
tf	502.42	K	Joback Method
vc	0.881	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	647.16	J/mol×K	792.02	Joback Method
cpg	660.53	J/mol×K	826.91	Joback Method
cpg	672.95	J/mol×K	861.80	Joback Method
cpg	684.45	J/mol×K	896.69	Joback Method
cpg	695.04	J/mol×K	931.58	Joback Method
cpg	704.77	J/mol×K	966.46	Joback Method
cpg	713.66	J/mol×K	1001.35	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=U321719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321719&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>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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