

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

Inchi:	InChI=1S/C13H16ClNO3/c1-2-9-18-12(16)7-8-15-13(17)10-3-5-11(14)6-4-10/h3-6H,2,7-9
InchiKey:	MRMFHSQHERDFJF-UHFFFAOYSA-N
Formula:	C13H16ClNO3
SMILES:	CCCOC(=O)CCNC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	269.72

## Physical Properties

Property code	Value	Unit	Source
gf	-124.02	kJ/mol	Joback Method
hf	-406.24	kJ/mol	Joback Method
hfus	36.76	kJ/mol	Joback Method
hvap	74.19	kJ/mol	Joback Method
log10ws	-3.46		Crippen Method
logp	2.413		Crippen Method
mvol	201.500	ml/mol	McGowan Method
pc	2345.09	kPa	Joback Method
rinpol	2181.00		NIST Webbook
rinpol	2181.00		NIST Webbook
tb	746.26	K	Joback Method
tc	959.99	K	Joback Method
tf	479.88	K	Joback Method
vc	0.769	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	538.84	J/mol×K	746.26	Joback Method
cpg	551.48	J/mol×K	781.88	Joback Method
cpg	563.22	J/mol×K	817.50	Joback Method
cpg	574.09	J/mol×K	853.12	Joback Method
cpg	584.10	J/mol×K	888.74	Joback Method
cpg	593.28	J/mol×K	924.37	Joback Method
cpg	601.66	J/mol×K	959.99	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321717&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321717&amp;Units=SI</a>
<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>

# 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>hvp:</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>rinp:</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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