

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

Inchi:	InChI=1S/C18H26ClNO3/c1-2-3-4-5-6-7-14-23-17(21)12-13-20-18(22)15-8-10-16(19)11-
InchiKey:	BTYTZIBBNKDRCF-UHFFFAOYSA-N
Formula:	C18H26ClNO3
SMILES:	CCCCCCCCOC(=O)CCNC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	339.86

## Physical Properties

Property code	Value	Unit	Source
gf	-81.92	kJ/mol	Joback Method
hf	-509.44	kJ/mol	Joback Method
hfus	49.71	kJ/mol	Joback Method
hvap	85.32	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	4.364		Crippen Method
mcvol	271.950	ml/mol	McGowan Method
pc	1543.92	kPa	Joback Method
rinpol	2705.00		NIST Webbook
tb	860.66	K	Joback Method
tc	1067.86	K	Joback Method
tf	536.23	K	Joback Method
vc	1.050	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.00	J/molxK	860.66	Joback Method
cpg	831.20	J/molxK	895.19	Joback Method
cpg	844.37	J/molxK	929.73	Joback Method
cpg	856.53	J/molxK	964.26	Joback Method
cpg	867.72	J/molxK	998.79	Joback Method
cpg	877.99	J/molxK	1033.32	Joback Method
cpg	887.36	J/molxK	1067.86	Joback Method

# Sources

<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=U321722&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321722&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>

# 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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