

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

Inchi:	InChI=1S/C22H34ClNO3/c1-2-3-4-5-6-7-8-9-10-11-18-27-21(25)16-17-24-22(26)19-12-1
InchiKey:	CIEGTMHJJZHPCN-UHFFFAOYSA-N
Formula:	C22H34ClNO3
SMILES:	CCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	395.96

## Physical Properties

Property code	Value	Unit	Source
gf	-48.24	kJ/mol	Joback Method
hf	-592.00	kJ/mol	Joback Method
hfus	60.07	kJ/mol	Joback Method
hvap	94.23	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	5.924		Crippen Method
mvol	328.310	ml/mol	McGowan Method
pc	1165.63	kPa	Joback Method
rinpol	3352.00		NIST Webbook
rinpol	3352.00		NIST Webbook
tb	952.18	K	Joback Method
tc	1166.90	K	Joback Method
tf	581.31	K	Joback Method
vc	1.274	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.39	J/mol×K	952.18	Joback Method
cpg	1069.62	J/mol×K	987.97	Joback Method
cpg	1083.64	J/mol×K	1023.75	Joback Method
cpg	1096.50	J/mol×K	1059.54	Joback Method
cpg	1108.27	J/mol×K	1095.32	Joback Method
cpg	1119.00	J/mol×K	1131.11	Joback Method
cpg	1128.73	J/mol×K	1166.90	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=U321726&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321726&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>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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