

# «beta»-Alanine, N-(4-fluorobenzoyl)-, pentadecyl ester

Inchi:	InChI=1S/C25H40FNO3/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-21-30-24(28)19-20-27-25(29)
InchiKey:	WSGJHBJRCRTBRA-UHFFFAOYSA-N
Formula:	C25H40FNO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	421.59

## Physical Properties

Property code	Value	Unit	Source
gf	-205.86	kJ/mol	Joback Method
hf	-834.29	kJ/mol	Joback Method
hfus	66.72	kJ/mol	Joback Method
hvap	95.70	kJ/mol	Joback Method
log10ws	-8.13		Crippen Method
logp	6.580		Crippen Method
mcvol	360.110	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
tb	982.66	K	Joback Method
tc	1204.27	K	Joback Method
tf	585.79	K	Joback Method
vc	1.411	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1219.80	J/molxK	982.66	Joback Method
cpg	1236.96	J/molxK	1019.60	Joback Method
cpg	1252.72	J/molxK	1056.53	Joback Method
cpg	1267.15	J/molxK	1093.47	Joback Method
cpg	1280.31	J/molxK	1130.40	Joback Method
cpg	1292.29	J/molxK	1167.34	Joback Method
cpg	1303.15	J/molxK	1204.27	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=U321766&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321766&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>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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