

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

Inchi:	InChI=1S/C14H18FNO3/c1-2-3-10-19-13(17)8-9-16-14(18)11-4-6-12(15)7-5-11/h4-7H,2-
InchiKey:	AMSNRKYUTPPQPR-UHFFFAOYSA-N
Formula:	C14H18FNO3
SMILES:	CCCCOC(=O)CCNC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	267.30

## Physical Properties

Property code	Value	Unit	Source
gf	-298.48	kJ/mol	Joback Method
hf	-607.25	kJ/mol	Joback Method
hfus	38.23	kJ/mol	Joback Method
hvap	71.22	kJ/mol	Joback Method
log10ws	-3.52		Crippen Method
logp	2.289		Crippen Method
mvol	205.120	ml/mol	McGowan Method
pc	2125.60	kPa	Joback Method
rinpol	2060.00		NIST Webbook
rinpol	2060.00		NIST Webbook
tb	730.98	K	Joback Method
tc	931.51	K	Joback Method
tf	461.82	K	Joback Method
vc	0.794	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	574.91	J/mol×K	730.98	Joback Method
cpg	588.47	J/mol×K	764.40	Joback Method
cpg	601.16	J/mol×K	797.82	Joback Method
cpg	612.99	J/mol×K	831.24	Joback Method
cpg	623.99	J/mol×K	864.66	Joback Method
cpg	634.19	J/mol×K	898.08	Joback Method
cpg	643.60	J/mol×K	931.51	Joback Method

# Sources

<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>
<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=U321756&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321756&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>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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