

# «beta»-Alanine, N-(3-fluorobenzoyl)-, propyl ester

Inchi:	InChI=1S/C13H16FNO3/c1-2-8-18-12(16)6-7-15-13(17)10-4-3-5-11(14)9-10/h3-5,9H,2,6
InchiKey:	JYZGENXNIZQTKS-UHFFFAOYSA-N
Formula:	C13H16FNO3
SMILES:	CCCOC(=O)CCNC(=O)c1cccc(F)c1
Mol. weight [g/mol]:	253.27

## Physical Properties

Property code	Value	Unit	Source
gf	-306.90	kJ/mol	Joback Method
hf	-586.61	kJ/mol	Joback Method
hfus	35.64	kJ/mol	Joback Method
hvap	68.99	kJ/mol	Joback Method
log10ws	-3.10		Crippen Method
logp	1.899		Crippen Method
mcvol	191.030	ml/mol	McGowan Method
pc	2327.03	kPa	Joback Method
rinpol	1942.00		NIST Webbook
rinpol	1942.00		NIST Webbook
tb	708.10	K	Joback Method
tc	910.62	K	Joback Method
tf	450.55	K	Joback Method
vc	0.739	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.81	J/molxK	708.10	Joback Method
cpg	534.94	J/molxK	741.85	Joback Method
cpg	547.22	J/molxK	775.61	Joback Method
cpg	558.68	J/molxK	809.36	Joback Method
cpg	569.34	J/molxK	843.11	Joback Method
cpg	579.22	J/molxK	876.87	Joback Method
cpg	588.34	J/molxK	910.62	Joback Method

# Sources

<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=U321933&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321933&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>
<b>Crippen Method:</b>	<a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</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>rinpola:</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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