

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

Inchi:	InChI=1S/C20H30FNO3/c1-2-3-4-5-6-7-8-9-16-25-19(23)14-15-22-20(24)17-10-12-18(21)
InchiKey:	HTEDKMSQOVAZGT-UHFFFAOYSA-N
Formula:	C20H30FNO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccc(F)cc1
Mol. weight [g/mol]:	351.46

## Physical Properties

Property code	Value	Unit	Source
gf	-247.96	kJ/mol	Joback Method
hf	-731.09	kJ/mol	Joback Method
hfus	53.77	kJ/mol	Joback Method
hvap	84.57	kJ/mol	Joback Method
log10ws	-6.03		Crippen Method
logp	4.630		Crippen Method
mvol	289.660	ml/mol	McGowan Method
pc	1327.14	kPa	Joback Method
rinpol	2669.00		NIST Webbook
rinpol	2669.00		NIST Webbook
tb	868.26	K	Joback Method
tc	1068.64	K	Joback Method
tf	529.44	K	Joback Method
vc	1.131	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	915.25	J/mol×K	868.26	Joback Method
cpg	930.70	J/mol×K	901.66	Joback Method
cpg	945.08	J/mol×K	935.05	Joback Method
cpg	958.41	J/mol×K	968.45	Joback Method
cpg	970.74	J/mol×K	1001.85	Joback Method
cpg	982.10	J/mol×K	1035.24	Joback Method
cpg	992.54	J/mol×K	1068.64	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=U321762&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321762&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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