

# «beta»-Alanine, N-(4-butylbenzoyl)-, heptyl ester

Inchi:	InChI=1S/C21H33NO3/c1-3-5-7-8-9-17-25-20(23)15-16-22-21(24)19-13-11-18(12-14-19)
InchiKey:	ARQXGAOKIWWROC-UHFFFAOYSA-N
Formula:	C21H33NO3
SMILES:	CCCCCCCOC(=O)CCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	347.49

## Physical Properties

Property code	Value	Unit	Source
gf	-44.73	kJ/mol	Joback Method
hf	-555.62	kJ/mol	Joback Method
hfus	53.28	kJ/mol	Joback Method
hvap	87.62	kJ/mol	Joback Method
log10ws	-6.09		Crippen Method
logp	4.663		Crippen Method
mcvol	301.980	ml/mol	McGowan Method
pc	1279.16	kPa	Joback Method
rinpol	2855.00		NIST Webbook
tb	891.87	K	Joback Method
tc	1097.18	K	Joback Method
tf	540.12	K	Joback Method
vc	1.169	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	967.75	J/molxK	891.87	Joback Method
cpg	983.80	J/molxK	926.09	Joback Method
cpg	998.70	J/molxK	960.31	Joback Method
cpg	1012.49	J/molxK	994.52	Joback Method
cpg	1025.22	J/molxK	1028.74	Joback Method
cpg	1036.92	J/molxK	1062.96	Joback Method
cpg	1047.64	J/molxK	1097.18	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321774&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321774&amp;Units=SI</a>
<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.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>

# 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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