

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

Inchi:	InChI=1S/C17H25NO3/c1-3-5-6-14-7-9-15(10-8-14)17(20)18-12-11-16(19)21-13-4-2/h7-
InchiKey:	MLXNMDBZKDIUHF-UHFFFAOYSA-N
Formula:	C17H25NO3
SMILES:	CCCCc1ccc(C(=O)NCCC(=O)OCCC)cc1
Mol. weight [g/mol]:	291.39

## Physical Properties

Property code	Value	Unit	Source
gf	-78.41	kJ/mol	Joback Method
hf	-473.06	kJ/mol	Joback Method
hfus	42.92	kJ/mol	Joback Method
hvap	78.71	kJ/mol	Joback Method
log10ws	-4.41		Crippen Method
logp	3.102		Crippen Method
mvol	245.620	ml/mol	McGowan Method
pc	1718.88	kPa	Joback Method
rinpol	2430.00		NIST Webbook
tb	800.35	K	Joback Method
tc	1003.35	K	Joback Method
tf	495.04	K	Joback Method
vc	0.945	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	733.33	J/mol×K	800.35	Joback Method
cpg	748.41	J/mol×K	834.18	Joback Method
cpg	762.47	J/mol×K	868.02	Joback Method
cpg	775.56	J/mol×K	901.85	Joback Method
cpg	787.69	J/mol×K	935.68	Joback Method
cpg	798.90	J/mol×K	969.52	Joback Method
cpg	809.22	J/mol×K	1003.35	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=U321768&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321768&amp;Units=SI</a>
<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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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