

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

Inchi:	InChI=1S/C16H23NO3/c1-3-5-12-20-15(18)10-11-17-16(19)14-8-6-13(4-2)7-9-14/h6-9H,
InchiKey:	FRJBNHLVHAKPLA-UHFFFAOYSA-N
Formula:	C16H23NO3
SMILES:	CCCCOC(=O)CCNC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]:	277.36

## Physical Properties

Property code	Value	Unit	Source
gf	-86.83	kJ/mol	Joback Method
hf	-452.42	kJ/mol	Joback Method
hfus	40.33	kJ/mol	Joback Method
hvap	76.49	kJ/mol	Joback Method
log10ws	-3.99		Crippen Method
logp	2.712		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1864.33	kPa	Joback Method
rinpol	2329.00		NIST Webbook
rinpol	2329.00		NIST Webbook
tb	777.47	K	Joback Method
tc	981.54	K	Joback Method
tf	483.77	K	Joback Method
vc	0.888	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.89	J/molxK	777.47	Joback Method
cpg	691.69	J/molxK	811.48	Joback Method
cpg	705.50	J/molxK	845.49	Joback Method
cpg	718.36	J/molxK	879.50	Joback Method
cpg	730.30	J/molxK	913.51	Joback Method
cpg	741.33	J/molxK	947.53	Joback Method
cpg	751.49	J/molxK	981.54	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=U321653&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321653&amp;Units=SI</a>

# Legend

<b>cp<sub>g</sub>:</b>	Ideal gas heat capacity
<b>g<sub>f</sub>:</b>	Standard Gibbs free energy of formation
<b>h<sub>f</sub>:</b>	Enthalpy of formation at standard conditions
<b>h<sub>fus</sub>:</b>	Enthalpy of fusion at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>ws:</b>	Log <sub>10</sub> of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rin<sub>pol</sub>:</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

Latest version available from:

<https://www.cheméo.com/cid/116-620-4/beta-Alanine-N-4-ethylbenzoyl-butyl-ester.pdf>

Generated by Cheméo on 2025-02-08 19:49:14.991026046 +0000 UTC m=+2252370.837951669.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.