

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

Inchi:	InChI=1S/C16H23NO3/c1-4-13-5-7-14(8-6-13)16(19)17-10-9-15(18)20-11-12(2)3/h5-8,12
InchiKey:	LMAJCEWWZVFOQQ-UHFFFAOYSA-N
Formula:	C16H23NO3
SMILES:	CCc1ccc(C(=O)NCCC(=O)OCC(C)C)cc1
Mol. weight [g/mol]:	277.36

## Physical Properties

Property code	Value	Unit	Source
gf	-89.27	kJ/mol	Joback Method
hf	-457.70	kJ/mol	Joback Method
hfus	36.81	kJ/mol	Joback Method
hvap	76.10	kJ/mol	Joback Method
log10ws	-3.75		Crippen Method
logp	2.568		Crippen Method
mcvol	231.530	ml/mol	McGowan Method
pc	1877.28	kPa	Joback Method
rinpol	2259.00		NIST Webbook
tb	777.03	K	Joback Method
tc	983.90	K	Joback Method
tf	468.77	K	Joback Method
vc	0.882	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	677.44	J/molxK	777.03	Joback Method
cpg	692.45	J/molxK	811.51	Joback Method
cpg	706.43	J/molxK	845.99	Joback Method
cpg	719.42	J/molxK	880.46	Joback Method
cpg	731.45	J/molxK	914.94	Joback Method
cpg	742.54	J/molxK	949.42	Joback Method
cpg	752.73	J/molxK	983.90	Joback Method

# Sources

<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=U321652&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321652&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.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>

# 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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