

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

Inchi:	InChI=1S/C19H29NO3/c1-3-5-6-7-8-15-23-18(21)13-14-20-19(22)17-11-9-16(4-2)10-12-
InchiKey:	SPEPUMXUEBSPRQ-UHFFFAOYSA-N
Formula:	C19H29NO3
SMILES:	CCCCCCCOC(=O)CCNC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]:	319.44

## Physical Properties

Property code	Value	Unit	Source
gf	-61.57	kJ/mol	Joback Method
hf	-514.34	kJ/mol	Joback Method
hfus	48.10	kJ/mol	Joback Method
hvap	83.16	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	3.882		Crippen Method
mvol	273.800	ml/mol	McGowan Method
pc	1474.75	kPa	Joback Method
rinpol	2620.00		NIST Webbook
rinpol	2620.00		NIST Webbook
tb	846.11	K	Joback Method
tc	1048.85	K	Joback Method
tf	517.58	K	Joback Method
vc	1.056	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.95	J/mol×K	846.11	Joback Method
cpg	864.52	J/mol×K	879.90	Joback Method
cpg	879.02	J/mol×K	913.69	Joback Method
cpg	892.47	J/mol×K	947.48	Joback Method
cpg	904.93	J/mol×K	981.27	Joback Method
cpg	916.42	J/mol×K	1015.06	Joback Method
cpg	926.98	J/mol×K	1048.85	Joback Method

# Sources

<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>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321655&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321655&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>

# 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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