

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

Inchi:	InChI=1S/C24H39NO3/c1-3-5-6-7-8-9-10-11-12-13-20-28-23(26)18-19-25-24(27)22-16-1
InchiKey:	HOQXHRXLSCVIBX-UHFFFAOYSA-N
Formula:	C24H39NO3
SMILES:	CCCCCCCCCCCCOC(=O)CCNC(=O)c1ccc(CC)cc1
Mol. weight [g/mol]:	389.57

## Physical Properties

Property code	Value	Unit	Source
gf	-19.47	kJ/mol	Joback Method
hf	-617.54	kJ/mol	Joback Method
hfus	61.05	kJ/mol	Joback Method
hvap	94.29	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	5.833		Crippen Method
mvol	344.250	ml/mol	McGowan Method
pc	1051.41	kPa	Joback Method
rinpol	3366.00		NIST Webbook
rinpol	3366.00		NIST Webbook
tb	960.51	K	Joback Method
tc	1175.99	K	Joback Method
tf	573.93	K	Joback Method
vc	1.337	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1150.88	J/mol×K	960.51	Joback Method
cpg	1167.76	J/mol×K	996.42	Joback Method
cpg	1183.34	J/mol×K	1032.34	Joback Method
cpg	1197.65	J/mol×K	1068.25	Joback Method
cpg	1210.76	J/mol×K	1104.16	Joback Method
cpg	1222.74	J/mol×K	1140.07	Joback Method
cpg	1233.63	J/mol×K	1175.99	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=U321660&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321660&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>h vap:</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>r in pol:</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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