

# «beta»-Alanine, N-(4-methylbenzoyl)-, undecyl ester

Inchi:	InChI=1S/C22H35NO3/c1-3-4-5-6-7-8-9-10-11-18-26-21(24)16-17-23-22(25)20-14-12-19
InchiKey:	NYKZGJGHRINBU-UHFFFAOYSA-N
Formula:	C22H35NO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	361.52

## Physical Properties

Property code	Value	Unit	Source
gf	-36.31	kJ/mol	Joback Method
hf	-576.26	kJ/mol	Joback Method
hfus	55.87	kJ/mol	Joback Method
hvap	89.84	kJ/mol	Joback Method
log10ws	-6.60		Crippen Method
logp	5.189		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
pc	1195.65	kPa	Joback Method
rinsol	3051.00		NIST Webbook
tb	914.75	K	Joback Method
tc	1122.55	K	Joback Method
tf	551.39	K	Joback Method
vc	1.224	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1028.20	J/mol×K	914.75	Joback Method
cpg	1044.50	J/mol×K	949.38	Joback Method
cpg	1059.61	J/mol×K	984.02	Joback Method
cpg	1073.57	J/mol×K	1018.65	Joback Method
cpg	1086.42	J/mol×K	1053.28	Joback Method
cpg	1098.21	J/mol×K	1087.91	Joback Method
cpg	1109.00	J/mol×K	1122.55	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321609&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321609&amp;Units=SI</a>
<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.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>

# 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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