

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

Inchi:	InChI=1S/C25H41NO3/c1-3-5-7-8-9-10-11-12-13-21-29-24(27)19-20-26-25(28)23-17-15
InchiKey:	HDORCROQNXCDDX-UHFFFAOYSA-N
Formula:	C25H41NO3
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccc(CCCC)cc1
Mol. weight [g/mol]:	403.60

## Physical Properties

Property code	Value	Unit	Source
gf	-11.05	kJ/mol	Joback Method
hf	-638.18	kJ/mol	Joback Method
hfus	63.64	kJ/mol	Joback Method
hvap	96.52	kJ/mol	Joback Method
log10ws	-7.76		Crippen Method
logp	6.223		Crippen Method
mcvol	358.340	ml/mol	McGowan Method
pc	988.88	kPa	Joback Method
tb	983.39	K	Joback Method
tc	1204.19	K	Joback Method
tf	585.20	K	Joback Method
vc	1.393	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1213.01	J/molxK	983.39	Joback Method
cpg	1230.24	J/molxK	1020.19	Joback Method
cpg	1246.07	J/molxK	1056.99	Joback Method
cpg	1260.58	J/molxK	1093.79	Joback Method
cpg	1273.84	J/molxK	1130.59	Joback Method
cpg	1285.91	J/molxK	1167.39	Joback Method
cpg	1296.85	J/molxK	1204.19	Joback Method

# Sources

<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=U321778&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321778&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>

# 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>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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