

# «beta»-Alanine, N-(3-methoxybenzoyl)-, dodecyl ester

Inchi:	InChI=1S/C23H37NO4/c1-3-4-5-6-7-8-9-10-11-12-18-28-22(25)16-17-24-23(26)20-14-13
InchiKey:	LYLYHUMCKPGXJH-UHFFFAOYSA-N
Formula:	C23H37NO4
SMILES:	CCCCCCCCCCCCOC(=O)CCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	391.54

## Physical Properties

Property code	Value	Unit	Source
gf	-132.89	kJ/mol	Joback Method
hf	-729.12	kJ/mol	Joback Method
hfus	59.65	kJ/mol	Joback Method
hvap	94.48	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	5.279		Crippen Method
mcvol	336.030	ml/mol	McGowan Method
pc	1107.42	kPa	Joback Method
tb	960.05	K	Joback Method
tc	1175.46	K	Joback Method
tf	584.89	K	Joback Method
vc	1.298	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.61	J/molxK	960.05	Joback Method
cpg	1134.57	J/molxK	995.95	Joback Method
cpg	1149.13	J/molxK	1031.85	Joback Method
cpg	1162.33	J/molxK	1067.76	Joback Method
cpg	1174.20	J/molxK	1103.66	Joback Method
cpg	1184.79	J/molxK	1139.56	Joback Method
cpg	1194.13	J/molxK	1175.46	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=U321715&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321715&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>mcvol:</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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