

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

Inchi:	InChI=1S/C17H25NO4/c1-3-4-5-6-12-22-16(19)10-11-18-17(20)14-8-7-9-15(13-14)21-2/
InchiKey:	ICBQEPSZEMDQMZ-UHFFFAOYSA-N
Formula:	C17H25NO4
SMILES:	CCCCCOC(=O)CCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	307.38

## Physical Properties

Property code	Value	Unit	Source
gf	-183.41	kJ/mol	Joback Method
hf	-605.28	kJ/mol	Joback Method
hfus	44.11	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-4.15		Crippen Method
logp	2.939		Crippen Method
mvol	251.490	ml/mol	McGowan Method
pc	1694.90	kPa	Joback Method
rinpol	2545.00		NIST Webbook
rinpol	2545.00		NIST Webbook
tb	822.77	K	Joback Method
tc	1025.84	K	Joback Method
tf	517.27	K	Joback Method
vc	0.963	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	761.56	J/mol×K	822.77	Joback Method
cpg	776.21	J/mol×K	856.62	Joback Method
cpg	789.80	J/mol×K	890.46	Joback Method
cpg	802.35	J/mol×K	924.31	Joback Method
cpg	813.88	J/mol×K	958.15	Joback Method
cpg	824.40	J/mol×K	992.00	Joback Method
cpg	833.92	J/mol×K	1025.84	Joback Method

# Sources

<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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=U321709&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321709&amp;Units=SI</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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