

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

Inchi:	InChI=1S/C16H23NO4/c1-3-4-5-11-21-15(18)9-10-17-16(19)13-7-6-8-14(12-13)20-2/h6-
InchiKey:	VHYNAJSUHWZOMZ-UHFFFAOYSA-N
Formula:	C16H23NO4
SMILES:	CCCCCOC(=O)CCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	293.36

## Physical Properties

Property code	Value	Unit	Source
gf	-191.83	kJ/mol	Joback Method
hf	-584.64	kJ/mol	Joback Method
hfus	41.52	kJ/mol	Joback Method
hvap	78.90	kJ/mol	Joback Method
log10ws	-3.73		Crippen Method
logp	2.548		Crippen Method
mvol	237.400	ml/mol	McGowan Method
pc	1837.26	kPa	Joback Method
rinpol	2446.00		NIST Webbook
rinpol	2446.00		NIST Webbook
tb	799.89	K	Joback Method
tc	1003.51	K	Joback Method
tf	506.00	K	Joback Method
vc	0.906	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	704.68	J/mol×K	799.89	Joback Method
cpg	719.08	J/mol×K	833.83	Joback Method
cpg	732.46	J/mol×K	867.76	Joback Method
cpg	744.84	J/mol×K	901.70	Joback Method
cpg	756.23	J/mol×K	935.64	Joback Method
cpg	766.63	J/mol×K	969.57	Joback Method
cpg	776.08	J/mol×K	1003.51	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=U321707&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321707&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.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>

# 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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