

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

Inchi:	InChI=1S/C13H17NO4/c1-3-18-12(15)7-8-14-13(16)10-5-4-6-11(9-10)17-2/h4-6,9H,3,7-8
InchiKey:	LWVCEYHCNMWYGU-UHFFFAOYSA-N
Formula:	C13H17NO4
SMILES:	CCOC(=O)CCNC(=O)c1cccc(OC)c1
Mol. weight [g/mol]:	251.28

## Physical Properties

Property code	Value	Unit	Source
gf	-217.09	kJ/mol	Joback Method
hf	-522.72	kJ/mol	Joback Method
hfus	33.75	kJ/mol	Joback Method
hvap	72.22	kJ/mol	Joback Method
log10ws	-2.47		Crippen Method
logp	1.378		Crippen Method
mvol	195.130	ml/mol	McGowan Method
pc	2391.19	kPa	Joback Method
rinpol	2147.00		NIST Webbook
rinpol	2147.00		NIST Webbook
tb	731.25	K	Joback Method
tc	939.96	K	Joback Method
tf	472.19	K	Joback Method
vc	0.739	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	539.99	J/mol×K	731.25	Joback Method
cpg	553.40	J/mol×K	766.04	Joback Method
cpg	565.91	J/mol×K	800.82	Joback Method
cpg	577.51	J/mol×K	835.61	Joback Method
cpg	588.22	J/mol×K	870.39	Joback Method
cpg	598.04	J/mol×K	905.18	Joback Method
cpg	606.99	J/mol×K	939.96	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U321703&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321703&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>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

Latest version available from:

<https://www.chemeo.com/cid/113-910-5/beta-Alanine-N-3-methoxybenzoyl-ethyl-ester.pdf>

Generated by Cheméo on 2024-04-28 02:15:38.765105472 +0000 UTC m=+16559787.685682790.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.