

# «beta»-Alanine, N-(4-methoxybenzoyl)-, nonyl ester

Inchi:	InChI=1S/C20H31NO4/c1-3-4-5-6-7-8-9-16-25-19(22)14-15-21-20(23)17-10-12-18(24-2)
InchiKey:	JZEHJCBVRWYXRS-UHFFFAOYSA-N
Formula:	C20H31NO4
SMILES:	CCCCCCCCCOC(=O)CCNC(=O)c1ccc(OC)cc1
Mol. weight [g/mol]:	349.46

## Physical Properties

Property code	Value	Unit	Source
gf	-158.15	kJ/mol	Joback Method
hf	-667.20	kJ/mol	Joback Method
hfus	51.88	kJ/mol	Joback Method
hvap	87.80	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.109		Crippen Method
mvol	293.760	ml/mol	McGowan Method
pc	1354.63	kPa	Joback Method
rinpol	2956.00		NIST Webbook
tb	891.41	K	Joback Method
tc	1096.98	K	Joback Method
tf	551.08	K	Joback Method
vc	1.131	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	937.10	J/mol×K	891.41	Joback Method
cpg	952.40	J/mol×K	925.67	Joback Method
cpg	966.51	J/mol×K	959.93	Joback Method
cpg	979.43	J/mol×K	994.19	Joback Method
cpg	991.21	J/mol×K	1028.45	Joback Method
cpg	1001.87	J/mol×K	1062.71	Joback Method
cpg	1011.44	J/mol×K	1096.98	Joback Method

# Sources

<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>
<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=U321826&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321826&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>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>rinpola:</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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