

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

<b>Inchi:</b>	InChI=1S/C20H31NO4/c1-3-4-5-6-7-8-9-15-25-19(22)13-14-21-20(23)17-11-10-12-18(16)
<b>InchiKey:</b>	ZEZWMDSDDKRFDN-UHFFFAOYSA-N
<b>Formula:</b>	C20H31NO4
<b>SMILES:</b>	CCCCCCCCCOC(=O)CCN=C(O)c1cccc(OC)c1
<b>Mol. weight [g/mol]:</b>	349.46

## Physical Properties

Property code	Value	Unit	Source
hf	-687.89	kJ/mol	Joback Method
hvap	94.69	kJ/mol	Joback Method
log10ws	-4.95		Crippen Method
logp	4.684		Crippen Method
mcvol	293.760	ml/mol	McGowan Method
pc	1274.60	kPa	Joback Method
rinpol	2885.00		NIST Webbook
rinpol	2885.00		NIST Webbook
tb	956.11	K	Joback Method
tc	1171.18	K	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.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=U321712&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U321712&amp;Units=SI</a>

## Legend

<b>hf:</b>	Enthalpy of formation 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>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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