

# «beta»-Alanine, N-cyclohexylcarbonyl-, nonyl ester

**Inchi:** InChI=1S/C19H35NO3/c1-2-3-4-5-6-7-11-16-23-18(21)14-15-20-19(22)17-12-9-8-10-13-  
**InchiKey:** ZBAQBBLXSSP-UHFFFAOYSA-N  
**Formula:** C19H35NO3  
**SMILES:** CCCCCCCCCOC(=O)CCN=C(O)C1CCCCC1  
**Mol. weight [g/mol]:** 325.49

## Physical Properties

Property code	Value	Unit	Source
hf	-705.77	kJ/mol	Joback Method
hvap	87.55	kJ/mol	Joback Method
log10ws	-5.27		Crippen Method
logp	5.207		Crippen Method
mcvol	286.700	ml/mol	McGowan Method
pc	1276.42	kPa	Joback Method
rinpol	2557.00		NIST Webbook
rinpol	2557.00		NIST Webbook
tb	898.70	K	Joback Method
tc	1103.79	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321966&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307I>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** 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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