

# «beta»-Alanine, N-capryloyl-, dodecyl ester

**Inchi:** InChI=1S/C23H45NO3/c1-3-5-7-9-10-11-12-13-15-17-21-27-23(26)19-20-24-22(25)18-16  
**InchiKey:** VMTBPLPXIAWETA-UHFFFAOYSA-N  
**Formula:** C23H45NO3  
**SMILES:** CCCCCCCCCCOC(=O)CCN=C(O)CCCCCCC  
**Mol. weight [g/mol]:** 383.61

## Physical Properties

Property code	Value	Unit	Source
hf	-842.65	kJ/mol	Joback Method
hvap	96.02	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	7.158		Crippen Method
mcvol	353.920	ml/mol	McGowan Method
pc	871.19	kPa	Joback Method
rinpol	2929.00		NIST Webbook
rinpol	2929.00		NIST Webbook
tb	970.67	K	Joback Method
tc	1195.73	K	Joback Method

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U321817&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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