

# L-Valine, N-(3-methylbenzoyl)-, pentadecyl ester

**Inchi:** InChI=1S/C28H47NO3/c1-5-6-7-8-9-10-11-12-13-14-15-16-17-21-32-28(31)26(23(2)3)29  
**InchiKey:** XBBZOEKHEPGWLQ-UHFFFAOYSA-N  
**Formula:** C28H47NO3  
**SMILES:** CCCCCCCCCCCCCCOC(=O)C(N=C(O)c1cccc(C)c1)C(C)C  
**Mol. weight [g/mol]:** 445.68

## Physical Properties

Property code	Value	Unit	Source
hf	-731.35	kJ/mol	Joback Method
hvap	109.31	kJ/mol	Joback Method
log10ws	-8.52		Crippen Method
logp	7.959		Crippen Method
mcvol	400.610	ml/mol	McGowan Method
pc	799.79	kPa	Joback Method
rinpol	3304.00		NIST Webbook
rinpol	3304.00		NIST Webbook
tb	1115.85	K	Joback Method
tc	1382.64	K	Joback Method

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**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)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=U346653&Units=SI>

## 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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