

# 1-Aminocyclopentanecarboxylic acid, N-(but-3-yn-1-yloxycarbonyl)-, tetradecyl ester

**Inchi:** InChI=1S/C25H43NO4/c1-3-5-7-8-9-10-11-12-13-14-15-18-22-29-23(27)25(19-16-17-20-  
**InchiKey:** HJPNKDDMFRMVRF-UHFFFAOYSA-N  
**Formula:** C25H43NO4  
**SMILES:** C#CCCOC(O)=NC1(C(=O)OCCCCCCCCCCCCCCC)CCCC1  
**Mol. weight [g/mol]:** 421.61

## Physical Properties

Property code	Value	Unit	Source
hf	-648.53	kJ/mol	Joback Method
hvap	101.85	kJ/mol	Joback Method
log10ws	-7.52		Crippen Method
logp	6.497		Crippen Method
mcvol	368.510	ml/mol	McGowan Method
pc	962.08	kPa	Joback Method
rinpol	2879.00		NIST Webbook
rinpol	2879.00		NIST Webbook
tb	1044.49	K	Joback Method
tc	1282.20	K	Joback Method

## Sources

**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=U392576&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)

## 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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