

# 1-Aminocyclopentanecarboxylic acid, N-(but-2-yn-1-yloxycarbonyl)-, decyl ester

**Inchi:** InChI=1S/C21H35NO4/c1-3-5-7-8-9-10-11-14-18-25-19(23)21(15-12-13-16-21)22-20(24)  
**InchiKey:** PQGYRJCYFMDSV-UHFFFAOYSA-N  
**Formula:** C21H35NO4  
**SMILES:** CC#CCOC(O)=NC1(C(=O)OCCCCCCCCCCC)CCCC1  
**Mol. weight [g/mol]:** 365.51

## Physical Properties

Property code	Value	Unit	Source
hf	-585.57	kJ/mol	Joback Method
hvap	95.24	kJ/mol	Joback Method
log10ws	-5.84		Crippen Method
logp	4.937		Crippen Method
mcvol	312.150	ml/mol	McGowan Method
pc	1250.38	kPa	Joback Method
rinpol	2579.00		NIST Webbook
rinpol	2579.00		NIST Webbook
tb	971.85	K	Joback Method
tc	1191.52	K	Joback Method

## Sources

**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=U392584&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## 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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