

# 1-Aminocyclopentanecarboxylic acid, N-(but-3-en-1-yloxycarbonyl)-, heptyl ester

**Inchi:** InChI=1S/C18H31NO4/c1-3-5-7-8-11-15-22-16(20)18(12-9-10-13-18)19-17(21)23-14-6-4  
**InchiKey:** BXBPLQGVBLHPTA-UHFFFAOYSA-N  
**Formula:** C18H31NO4  
**SMILES:** C=CCCOC(O)=NC1(C(=O)OCCCCCCC)CCCC1  
**Mol. weight [g/mol]:** 325.44

## Physical Properties

Property code	Value	Unit	Source
hf	-670.52	kJ/mol	Joback Method
hvap	85.74	kJ/mol	Joback Method
log10ws	-4.65		Crippen Method
logp	4.319		Crippen Method
mcvol	274.180	ml/mol	McGowan Method
pc	1415.44	kPa	Joback Method
tb	890.89	K	Joback Method
tc	1096.53	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=U392595&Units=SI>

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient

**mcvol:** McGowan's characteristic volume  
**pc:** Critical Pressure  
**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature

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