# 1-Aminocyclopentanecarboxylic acid, N-(2-methoxyethoxycarbonyl)-, heptyl ester

**Inchi:** InChI=1S/C17H31NO5/c1-3-4-5-6-9-12-22-15(19)17(10-7-8-11-17)18-16(20)23-14-13-21

**InchiKey:** WQVKUDFVNODZLQ-UHFFFAOYSA-N

**Formula:** C17H31NO5

**SMILES:** CCCCCCCOC(=O)C1(N=C(O)OCCOC)CCCC1

**Mol. weight [g/mol]:** 329.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -907.53 | kJ/mol | Joback Method |
| hvap | 86.59 | kJ/mol | Joback Method |
| log10ws | -3.46 | | Crippen Method |
| logp | 3.390 | | Crippen Method |
| mcvol | 270.260 | ml/mol | McGowan Method |
| pc | 1455.68 | kPa | Joback Method |
| rinpol | 2218.00 | | NIST Webbook |
| tb | 893.75 | K | Joback Method |
| tc | 1098.92 | K | Joback Method |

## Sources

**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws

**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=U392540&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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |