# 1-Aminocyclopentanecarboxylic acid, N-(vinyloxycarbonyl)-, heptyl ester

**Inchi:** InChI=1S/C16H27NO4/c1-3-5-6-7-10-13-21-14(18)16(11-8-9-12-16)17-15(19)20-4-2/h4H

**InchiKey:** LQGNZKYPFKIMBV-UHFFFAOYSA-N

**Formula:** C16H27NO4

**SMILES:** C=COC(=O)NC1(C(=O)OCCCCCCC)CCCC1

**Mol. weight [g/mol]:** 297.39

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -175.71 | kJ/mol | Joback Method |
| hf | -608.55 | kJ/mol | Joback Method |
| hfus | 34.23 | kJ/mol | Joback Method |
| hvap | 74.39 | kJ/mol | Joback Method |
| log10ws | -4.77 | | Crippen Method |
| logp | 3.682 | | Crippen Method |
| mcvol | 246.000 | ml/mol | McGowan Method |
| pc | 1762.45 | kPa | Joback Method |
| rinpol | 1990.00 | | NIST Webbook |
| rinpol | 1990.00 | | NIST Webbook |
| tb | 780.43 | K | Joback Method |
| tc | 981.61 | K | Joback Method |
| tf | 500.10 | K | Joback Method |
| vc | 0.934 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 755.72 | J/mol×K | 780.43 | Joback Method |
| cpg | 772.94 | J/mol×K | 813.96 | Joback Method |
| cpg | 789.49 | J/mol×K | 847.49 | Joback Method |
| cpg | 805.46 | J/mol×K | 881.02 | Joback Method |
| cpg | 820.94 | J/mol×K | 914.55 | Joback Method |
| cpg | 836.02 | J/mol×K | 948.08 | Joback Method |
| cpg | 850.81 | J/mol×K | 981.61 | Joback Method |

# Sources

| | |
|---|---|
| **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=U392607&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion 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 |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |