# 1-Aminocyclopentanecarboxylic acid, 3-chloropropoxycarbonyl-, heptyl ester

**Inchi:** InChI=1S/C17H30ClNO4/c1-2-3-4-5-8-13-22-15(20)17(10-6-7-11-17)19-16(21)23-14-9-1

**InchiKey:** KPJIYUYOZUIECT-UHFFFAOYSA-N

**Formula:** C17H30ClNO4

**SMILES:** CCCCCCCOC(=O)C1(NC(=O)OCCCCl)CCCC1

**Mol. weight [g/mol]:** 347.88

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -267.06 | kJ/mol | Joback Method |
| hf | -770.36 | kJ/mol | Joback Method |
| hfus | 42.29 | kJ/mol | Joback Method |
| hvap | 81.67 | kJ/mol | Joback Method |
| log10ws | -4.99 | | Crippen Method |
| logp | 4.168 | | Crippen Method |
| mcvol | 276.630 | ml/mol | McGowan Method |
| pc | 1529.46 | kPa | Joback Method |
| rinpol | 2362.00 | | NIST Webbook |
| rinpol | 2362.00 | | NIST Webbook |
| tb | 844.06 | K | Joback Method |
| tc | 1047.37 | K | Joback Method |
| tf | 543.05 | K | Joback Method |
| vc | 1.058 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 870.73 | J/mol×K | 844.06 | Joback Method |
| cpg | 888.28 | J/mol×K | 877.94 | Joback Method |
| cpg | 905.23 | J/mol×K | 911.83 | Joback Method |
| cpg | 921.67 | J/mol×K | 945.71 | Joback Method |
| cpg | 937.70 | J/mol×K | 979.60 | Joback Method |
| cpg | 953.42 | J/mol×K | 1013.48 | Joback Method |
| cpg | 968.93 | J/mol×K | 1047.37 | 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=U392625&Units=SI |

# 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 |