# DL-Alanine, N-methyl-N-(3-chloropropoxycarbonyl)-, hexyl ester

**Inchi:** InChI=1S/C14H26ClNO4/c1-4-5-6-7-10-19-13(17)12(2)16(3)14(18)20-11-8-9-15/h12H,4-
**InchiKey:** ALVHZDRXLQHAQG-UHFFFAOYSA-N
**Formula:** C14H26ClNO4
**SMILES:** CCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
**Mol. weight [g/mol]:** 307.81

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -304.43 | kJ/mol | Joback Method |
| hf | -775.38 | kJ/mol | Joback Method |
| hfus | 41.28 | kJ/mol | Joback Method |
| hvap | 71.11 | kJ/mol | Joback Method |
| log10ws | -3.22 | | Crippen Method |
| logp | 3.196 | | Crippen Method |
| mcvol | 245.220 | ml/mol | McGowan Method |
| pc | 1598.72 | kPa | Joback Method |
| rinpol | 2010.00 | | NIST Webbook |
| rinpol | 2010.00 | | NIST Webbook |
| tb | 721.73 | K | Joback Method |
| tc | 903.95 | K | Joback Method |
| tf | 439.25 | K | Joback Method |
| vc | 0.928 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 693.57 | J/mol×K | 721.73 | Joback Method |
| cpg | 708.82 | J/mol×K | 752.10 | Joback Method |
| cpg | 723.24 | J/mol×K | 782.47 | Joback Method |
| cpg | 736.85 | J/mol×K | 812.84 | Joback Method |
| cpg | 749.66 | J/mol×K | 843.21 | Joback Method |
| cpg | 761.67 | J/mol×K | 873.58 | Joback Method |
| cpg | 772.91 | J/mol×K | 903.95 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392778&Units=SI |
| **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 |

# Legend

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|---|---|
| **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 |