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

**Inchi:** InChI=1S/C22H42ClNO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-18-27-21(25)20(2)24(3)22(2

**InchiKey:** VEABIJQMWXVRMH-UHFFFAOYSA-N

**Formula:** C22H42ClNO4

**SMILES:** CCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl

**Mol. weight [g/mol]:** 420.03

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -237.07 | kJ/mol | Joback Method |
| hf | -940.50 | kJ/mol | Joback Method |
| hfus | 62.00 | kJ/mol | Joback Method |
| hvap | 88.92 | kJ/mol | Joback Method |
| log10ws | -6.57 | | Crippen Method |
| logp | 6.317 | | Crippen Method |
| mcvol | 357.940 | ml/mol | McGowan Method |
| pc | 935.77 | kPa | Joback Method |
| rinpol | 2769.00 | | NIST Webbook |
| rinpol | 2769.00 | | NIST Webbook |
| tb | 904.77 | K | Joback Method |
| tc | 1108.02 | K | Joback Method |
| tf | 529.41 | K | Joback Method |
| vc | 1.377 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1167.81 | J/mol×K | 904.77 | Joback Method |
| cpg | 1186.21 | J/mol×K | 938.65 | Joback Method |
| cpg | 1203.29 | J/mol×K | 972.52 | Joback Method |
| cpg | 1219.09 | J/mol×K | 1006.40 | Joback Method |
| cpg | 1233.66 | J/mol×K | 1040.27 | Joback Method |
| cpg | 1247.02 | J/mol×K | 1074.15 | Joback Method |
| cpg | 1259.22 | J/mol×K | 1108.02 | Joback Method |

# Sources

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|---|---|
| **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=U392786&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |