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

**Inchi:** InChI=1S/C23H44ClNO4/c1-4-5-6-7-8-9-10-11-12-13-14-15-16-19-28-22(26)21(2)25(3)2
**InchiKey:** NRLOBYKKONJHMO-UHFFFAOYSA-N
**Formula:** C23H44ClNO4
**SMILES:** CCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCl
**Mol. weight [g/mol]:** 434.05

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -228.65 | kJ/mol | Joback Method |
| hf | -961.14 | kJ/mol | Joback Method |
| hfus | 64.60 | kJ/mol | Joback Method |
| hvap | 91.14 | kJ/mol | Joback Method |
| log10ws | -6.99 | | Crippen Method |
| logp | 6.707 | | Crippen Method |
| mcvol | 372.030 | ml/mol | McGowan Method |
| pc | 883.14 | kPa | Joback Method |
| rinpol | 2868.00 | | NIST Webbook |
| rinpol | 2868.00 | | NIST Webbook |
| tb | 927.65 | K | Joback Method |
| tc | 1137.36 | K | Joback Method |
| tf | 540.68 | K | Joback Method |
| vc | 1.433 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1230.29 | J/mol×K | 927.65 | Joback Method |
| cpg | 1249.17 | J/mol×K | 962.60 | Joback Method |
| cpg | 1266.63 | J/mol×K | 997.55 | Joback Method |
| cpg | 1282.71 | J/mol×K | 1032.51 | Joback Method |
| cpg | 1297.46 | J/mol×K | 1067.46 | Joback Method |
| cpg | 1310.93 | J/mol×K | 1102.41 | Joback Method |
| cpg | 1323.16 | J/mol×K | 1137.36 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392787&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |