# DL-Valine, N-methyl-N-(3-chloropropoxycarbonyl)-, undecyl ester

**Inchi:** InChI=1S/C21H40ClNO4/c1-5-6-7-8-9-10-11-12-13-16-26-20(24)19(18(2)3)23(4)21(25)2
**InchiKey:** QLKPDDHXROUQQJ-UHFFFAOYSA-N
**Formula:** C21H40ClNO4
**SMILES:** CCCCCCCCCCCOC(=O)C(C(C)C)N(C)C(=O)OCCCCl
**Mol. weight [g/mol]:** 406.00

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -247.93 | kJ/mol | Joback Method |
| hf | -925.14 | kJ/mol | Joback Method |
| hfus | 55.89 | kJ/mol | Joback Method |
| hvap | 86.30 | kJ/mol | Joback Method |
| log10ws | -5.91 | | Crippen Method |
| logp | 5.782 | | Crippen Method |
| mcvol | 343.850 | ml/mol | McGowan Method |
| pc | 998.28 | kPa | Joback Method |
| rinpol | 2600.00 | | NIST Webbook |
| rinpol | 2600.00 | | NIST Webbook |
| tb | 881.45 | K | Joback Method |
| tc | 1079.29 | K | Joback Method |
| tf | 503.14 | K | Joback Method |
| vc | 1.315 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1106.35 | J/mol×K | 881.45 | Joback Method |
| cpg | 1124.29 | J/mol×K | 914.42 | Joback Method |
| cpg | 1140.99 | J/mol×K | 947.40 | Joback Method |
| cpg | 1156.49 | J/mol×K | 980.37 | Joback Method |
| cpg | 1170.81 | J/mol×K | 1013.34 | Joback Method |
| cpg | 1184.00 | J/mol×K | 1046.32 | Joback Method |
| cpg | 1196.08 | J/mol×K | 1079.29 | Joback Method |

# Sources

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|---|---|
| **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=U392981&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 |