# DL-Valine, N-methyl-N-decyloxycarbonyl-, nonyl ester

**Inchi:** InChI=1S/C26H51NO4/c1-6-8-10-12-14-16-18-20-22-31-26(29)27(5)24(23(3)4)25(28)30-

**InchiKey:** WYXDSEYLZAHMJZ-UHFFFAOYSA-N

**Formula:** C26H51NO4

**SMILES:** CCCCCCCCCCOC(=O)N(C)C(C(=O)OCCCCCCCCC)C(C)C

**Mol. weight [g/mol]:** 441.69

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -193.90 | kJ/mol | Joback Method |
| hf | -1012.60 | kJ/mol | Joback Method |
| hfus | 64.65 | kJ/mol | Joback Method |
| hvap | 93.05 | kJ/mol | Joback Method |
| log10ws | -7.85 | | Crippen Method |
| logp | 7.514 | | Crippen Method |
| mcvol | 402.060 | ml/mol | McGowan Method |
| pc | 768.19 | kPa | Joback Method |
| rinpol | 2825.00 | | NIST Webbook |
| rinpol | 2825.00 | | NIST Webbook |
| tb | 958.42 | K | Joback Method |
| tc | 1180.17 | K | Joback Method |
| tf | 529.57 | K | Joback Method |
| vc | 1.546 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1390.97 | J/mol×K | 958.42 | Joback Method |
| cpg | 1412.29 | J/mol×K | 995.38 | Joback Method |
| cpg | 1431.89 | J/mol×K | 1032.34 | Joback Method |
| cpg | 1449.83 | J/mol×K | 1069.30 | Joback Method |
| cpg | 1466.16 | J/mol×K | 1106.26 | Joback Method |
| cpg | 1480.95 | J/mol×K | 1143.22 | Joback Method |
| cpg | 1494.27 | J/mol×K | 1180.17 | 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=U392926&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 |

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