# l-Valine, N-pivaloyl-, methyl ester

**Inchi:** InChI=1S/C11H21NO3/c1-7(2)8(9(13)15-6)12-10(14)11(3,4)5/h7-8H,1-6H3,(H,12,14)
**InchiKey:** ZOMUUMHLEGAWIX-UHFFFAOYSA-N
**Formula:** C11H21NO3
**SMILES:** COC(=O)C(NC(=O)C(C)(C)C)C(C)C
**Mol. weight [g/mol]:** 215.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -233.75 | kJ/mol | Joback Method |
| hf | -593.59 | kJ/mol | Joback Method |
| hfus | 19.27 | kJ/mol | Joback Method |
| hvap | 60.35 | kJ/mol | Joback Method |
| log10ws | -1.88 | | Crippen Method |
| logp | 1.346 | | Crippen Method |
| mcvol | 184.840 | ml/mol | McGowan Method |
| pc | 2231.30 | kPa | Joback Method |
| rinpol | 1343.00 | | NIST Webbook |
| rinpol | 1343.00 | | NIST Webbook |
| tb | 627.30 | K | Joback Method |
| tc | 824.24 | K | Joback Method |
| tf | 360.90 | K | Joback Method |
| vc | 0.694 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 496.08 | J/mol×K | 627.30 | Joback Method |
| cpg | 511.25 | J/mol×K | 660.12 | Joback Method |
| cpg | 525.57 | J/mol×K | 692.95 | Joback Method |
| cpg | 539.05 | J/mol×K | 725.77 | Joback Method |
| cpg | 551.72 | J/mol×K | 758.59 | Joback Method |
| cpg | 563.62 | J/mol×K | 791.42 | Joback Method |
| cpg | 574.76 | J/mol×K | 824.24 | 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=U299743&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 |