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

**Inchi:** InChI=1S/C9H17NO3/c1-6(7(11)13-5)10-8(12)9(2,3)4/h6H,1-5H3,(H,10,12)
**InchiKey:** OTUZHOXNCVOSAC-UHFFFAOYSA-N
**Formula:** C9H17NO3
**SMILES:** COC(=O)C(C)NC(=O)C(C)(C)C
**Mol. weight [g/mol]:** 187.24

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -248.15 | kJ/mol | Joback Method |
| hf | -547.03 | kJ/mol | Joback Method |
| hfus | 17.61 | kJ/mol | Joback Method |
| hvap | 56.28 | kJ/mol | Joback Method |
| log10ws | -1.29 | | Crippen Method |
| logp | 0.710 | | Crippen Method |
| mcvol | 156.660 | ml/mol | McGowan Method |
| pc | 2676.31 | kPa | Joback Method |
| rinpol | 1215.00 | | NIST Webbook |
| rinpol | 1215.00 | | NIST Webbook |
| tb | 581.98 | K | Joback Method |
| tc | 780.42 | K | Joback Method |
| tf | 353.36 | K | Joback Method |
| vc | 0.588 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 396.49 | J/mol×K | 581.98 | Joback Method |
| cpg | 410.14 | J/mol×K | 615.05 | Joback Method |
| cpg | 423.03 | J/mol×K | 648.13 | Joback Method |
| cpg | 435.19 | J/mol×K | 681.20 | Joback Method |
| cpg | 446.63 | J/mol×K | 714.27 | Joback Method |
| cpg | 457.38 | J/mol×K | 747.34 | Joback Method |
| cpg | 467.46 | J/mol×K | 780.42 | 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=U299741&Units=SI |

# 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 |