# l-Alanine, N-(2-fluorobenzoyl)-, methyl ester

**Inchi:** InChI=1S/C11H12FNO3/c1-7(11(15)16-2)13-10(14)8-5-3-4-6-9(8)12/h3-7H,1-2H3,(H,13,
**InchiKey:** HTMLUNCVOSASAC-UHFFFAOYSA-N
**Formula:** C11H12FNO3
**SMILES:** COC(=O)C(C)NC(=O)c1ccccc1F
**Mol. weight [g/mol]:** 225.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -326.18 | kJ/mol | Joback Method |
| hf | -550.61 | kJ/mol | Joback Method |
| hfus | 26.94 | kJ/mol | Joback Method |
| hvap | 64.15 | kJ/mol | Joback Method |
| log10ws | -2.38 | | Crippen Method |
| logp | 1.117 | | Crippen Method |
| mcvol | 162.850 | ml/mol | McGowan Method |
| pc | 2850.52 | kPa | Joback Method |
| rinpol | 1602.00 | | NIST Webbook |
| rinpol | 1602.00 | | NIST Webbook |
| tb | 661.90 | K | Joback Method |
| tc | 873.55 | K | Joback Method |
| tf | 413.01 | K | Joback Method |
| vc | 0.621 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 419.95 | J/mol×K | 661.90 | Joback Method |
| cpg | 432.27 | J/mol×K | 697.18 | Joback Method |
| cpg | 443.78 | J/mol×K | 732.45 | Joback Method |
| cpg | 454.49 | J/mol×K | 767.73 | Joback Method |
| cpg | 464.42 | J/mol×K | 803.00 | Joback Method |
| cpg | 473.58 | J/mol×K | 838.28 | Joback Method |
| cpg | 482.00 | J/mol×K | 873.55 | 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=U299619&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 |