# D-Alanine, N-(2,4-difluorobenzoyl)-, ethyl ester

**Inchi:** InChI=1S/C12H13F2NO3/c1-3-18-12(17)7(2)15-11(16)9-5-4-8(13)6-10(9)14/h4-7H,3H2,1
**InchiKey:** SPWLYEZCDHNCAK-UHFFFAOYSA-N
**Formula:** C12H13F2NO3
**SMILES:** CCOC(=O)C(C)NC(=O)c1ccc(F)cc1F
**Mol. weight [g/mol]:** 257.23

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -522.20 | kJ/mol | Joback Method |
| hf | -778.83 | kJ/mol | Joback Method |
| hfus | 32.22 | kJ/mol | Joback Method |
| hvap | 66.22 | kJ/mol | Joback Method |
| log10ws | -3.13 | | Crippen Method |
| logp | 1.646 | | Crippen Method |
| mcvol | 178.710 | ml/mol | McGowan Method |
| pc | 2429.05 | kPa | Joback Method |
| rinpol | 1687.00 | | NIST Webbook |
| rinpol | 1687.00 | | NIST Webbook |
| tb | 689.03 | K | Joback Method |
| tc | 890.27 | K | Joback Method |
| tf | 437.39 | K | Joback Method |
| vc | 0.695 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 477.36 | J/mol×K | 689.03 | Joback Method |
| cpg | 489.54 | J/mol×K | 722.57 | Joback Method |
| cpg | 500.94 | J/mol×K | 756.11 | Joback Method |
| cpg | 511.59 | J/mol×K | 789.65 | Joback Method |
| cpg | 521.50 | J/mol×K | 823.19 | Joback Method |
| cpg | 530.67 | J/mol×K | 856.73 | Joback Method |
| cpg | 539.12 | J/mol×K | 890.27 | Joback Method |

# Sources

| | |
|---|---|
| **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=U348456&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 |