# D-Alanine, N-(3-chloro-2-fluorobenzoyl)-, isobutyl ester

**Inchi:** InChI=1S/C14H17ClFNO3/c1-8(2)7-20-14(19)9(3)17-13(18)10-5-4-6-11(15)12(10)16/h4-

**InchiKey:** FAQBVVBBADVRJR-UHFFFAOYSA-N

**Formula:** C14H17ClFNO3

**SMILES:** CC(C)COC(=O)C(C)NC(=O)c1cccc(Cl)c1F

**Mol. weight [g/mol]:** 301.74

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -324.92 | kJ/mol | Joback Method |
| hf | -645.02 | kJ/mol | Joback Method |
| hfus | 34.99 | kJ/mol | Joback Method |
| hvap | 75.49 | kJ/mol | Joback Method |
| log10ws | -4.08 | | Crippen Method |
| logp | 2.797 | | Crippen Method |
| mcvol | 217.360 | ml/mol | McGowan Method |
| pc | 2056.76 | kPa | Joback Method |
| rinpol | 2078.00 | | NIST Webbook |
| tb | 772.51 | K | Joback Method |
| tc | 983.54 | K | Joback Method |
| tf | 474.26 | K | Joback Method |
| vc | 0.832 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 600.11 | J/mol×K | 772.51 | Joback Method |
| cpg | 612.90 | J/mol×K | 807.68 | Joback Method |
| cpg | 624.76 | J/mol×K | 842.85 | Joback Method |
| cpg | 635.70 | J/mol×K | 878.02 | Joback Method |
| cpg | 645.74 | J/mol×K | 913.19 | Joback Method |
| cpg | 654.91 | J/mol×K | 948.36 | Joback Method |
| cpg | 663.23 | J/mol×K | 983.54 | Joback Method |

# Sources

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|---|---|
| **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=U348335&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |