# D-Alanine, N-(4-anisoyl)-, hexyl ester

**Inchi:** InChI=1S/C17H25NO4/c1-4-5-6-7-12-22-17(20)13(2)18-16(19)14-8-10-15(21-3)11-9-14/h
**InchiKey:** GXNHEWVYLZFWCF-UHFFFAOYSA-N
**Formula:** C17H25NO4
**SMILES:** CCCCCCOC(=O)C(C)NC(=O)c1ccc(OC)cc1
**Mol. weight [g/mol]:** 307.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -185.85 | kJ/mol | Joback Method |
| hf | -610.56 | kJ/mol | Joback Method |
| hfus | 40.59 | kJ/mol | Joback Method |
| hvap | 80.73 | kJ/mol | Joback Method |
| log10ws | -4.26 | | Crippen Method |
| logp | 2.937 | | Crippen Method |
| mcvol | 251.490 | ml/mol | McGowan Method |
| pc | 1706.12 | kPa | Joback Method |
| rinpol | 2402.00 | | NIST Webbook |
| tb | 822.33 | K | Joback Method |
| tc | 1027.63 | K | Joback Method |
| tf | 502.27 | K | Joback Method |
| vc | 0.957 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 762.10 | J/mol×K | 822.33 | Joback Method |
| cpg | 776.91 | J/mol×K | 856.55 | Joback Method |
| cpg | 790.62 | J/mol×K | 890.76 | Joback Method |
| cpg | 803.26 | J/mol×K | 924.98 | Joback Method |
| cpg | 814.83 | J/mol×K | 959.20 | Joback Method |
| cpg | 825.37 | J/mol×K | 993.42 | Joback Method |
| cpg | 834.88 | J/mol×K | 1027.63 | 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=U348491&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 |