# D-Alanine, N-(4-ethylbenzoyl)-, dodecyl ester

**Inchi:** InChI=1S/C24H39NO3/c1-4-6-7-8-9-10-11-12-13-14-19-28-24(27)20(3)25-23(26)22-17-1
**InchiKey:** WDMIBDXWSLHAIR-UHFFFAOYSA-N
**Formula:** C24H39NO3
**SMILES:** CCCCCCCCCCCCOC(=O)C(C)NC(=O)c1ccc(CC)cc1
**Mol. weight [g/mol]:** 389.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -21.91 | kJ/mol | Joback Method |
| hf | -622.82 | kJ/mol | Joback Method |
| hfus | 57.53 | kJ/mol | Joback Method |
| hvap | 93.91 | kJ/mol | Joback Method |
| log10ws | -7.45 | | Crippen Method |
| logp | 5.831 | | Crippen Method |
| mcvol | 344.250 | ml/mol | McGowan Method |
| pc | 1056.88 | kPa | Joback Method |
| rinpol | 3029.00 | | NIST Webbook |
| tb | 960.07 | K | Joback Method |
| tc | 1175.65 | K | Joback Method |
| tf | 558.93 | K | Joback Method |
| vc | 1.331 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1151.27 | J/mol×K | 960.07 | Joback Method |
| cpg | 1168.12 | J/mol×K | 996.00 | Joback Method |
| cpg | 1183.64 | J/mol×K | 1031.93 | Joback Method |
| cpg | 1197.88 | J/mol×K | 1067.86 | Joback Method |
| cpg | 1210.91 | J/mol×K | 1103.79 | Joback Method |
| cpg | 1222.79 | J/mol×K | 1139.72 | Joback Method |
| cpg | 1233.57 | J/mol×K | 1175.65 | 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=U354093&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 |