# D-Alanine, N-neopentyloxycarbonyl-, hexyl ester

**Inchi:** InChI=1S/C15H29NO4/c1-6-7-8-9-10-19-13(17)12(2)16-14(18)20-11-15(3,4)5/h12H,6-11

**InchiKey:** NKUZRLRYPFTVJC-UHFFFAOYSA-N

**Formula:** C15H29NO4

**SMILES:** CCCCCCOC(=O)C(C)NC(=O)OCC(C)(C)C

**Mol. weight [g/mol]:** 287.40

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -302.63 | kJ/mol | Joback Method |
| hf | -803.09 | kJ/mol | Joback Method |
| hfus | 34.34 | kJ/mol | Joback Method |
| hvap | 72.05 | kJ/mol | Joback Method |
| log10ws | -3.86 | | Crippen Method |
| logp | 3.271 | | Crippen Method |
| mcvol | 247.070 | ml/mol | McGowan Method |
| pc | 1567.23 | kPa | Joback Method |
| rinpol | 1846.00 | | NIST Webbook |
| tb | 741.68 | K | Joback Method |
| tc | 929.19 | K | Joback Method |
| tf | 443.21 | K | Joback Method |
| vc | 0.942 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 739.80 | J/mol×K | 741.68 | Joback Method |
| cpg | 755.98 | J/mol×K | 772.93 | Joback Method |
| cpg | 771.24 | J/mol×K | 804.18 | Joback Method |
| cpg | 785.59 | J/mol×K | 835.43 | Joback Method |
| cpg | 799.06 | J/mol×K | 866.69 | Joback Method |
| cpg | 811.67 | J/mol×K | 897.94 | Joback Method |
| cpg | 823.44 | J/mol×K | 929.19 | 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=U347764&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 |