# D-Alanine, N-propargyloxycarbonyl-, tridecyl ester

**Inchi:** InChI=1S/C20H35NO4/c1-4-6-7-8-9-10-11-12-13-14-15-17-24-19(22)18(3)21-20(23)25-1
**InchiKey:** MZHDDJPJZGRJBZ-UHFFFAOYSA-N
**Formula:** C20H35NO4
**SMILES:** C#CCOC(=O)NC(C)C(=O)OCCCCCCCCCCCCC
**Mol. weight [g/mol]:** 353.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -40.30 | kJ/mol | Joback Method |
| hf | -605.64 | kJ/mol | Joback Method |
| hfus | 57.68 | kJ/mol | Joback Method |
| hvap | 84.33 | kJ/mol | Joback Method |
| log10ws | -5.99 | | Crippen Method |
| logp | 4.589 | | Crippen Method |
| mcvol | 308.920 | ml/mol | McGowan Method |
| pc | 1208.15 | kPa | Joback Method |
| rinpol | 2432.00 | | NIST Webbook |
| tb | 849.43 | K | Joback Method |
| tc | 1042.93 | K | Joback Method |
| tf | 544.11 | K | Joback Method |
| vc | 1.194 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 976.56 | J/mol×K | 849.43 | Joback Method |
| cpg | 993.34 | J/mol×K | 881.68 | Joback Method |
| cpg | 1009.05 | J/mol×K | 913.93 | Joback Method |
| cpg | 1023.72 | J/mol×K | 946.18 | Joback Method |
| cpg | 1037.36 | J/mol×K | 978.43 | Joback Method |
| cpg | 1050.01 | J/mol×K | 1010.68 | Joback Method |
| cpg | 1061.70 | J/mol×K | 1042.93 | 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=U347744&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 |