# DL-Alanine, N-methyl-N-(byt-4-en-1-yloxycarbonyl)-, dodecyl ester

**Inchi:** InChI=1S/C21H39NO4/c1-5-7-9-10-11-12-13-14-15-16-18-25-20(23)19(3)22(4)21(24)26-
**InchiKey:** LVRUYSBHTNCPOE-UHFFFAOYSA-N
**Formula:** C21H39NO4
**SMILES:** C=CCCOC(=O)N(C)C(C)C(=O)OCCCCCCCCCCCC
**Mol. weight [g/mol]:** 369.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -145.72 | kJ/mol | Joback Method |
| hf | -778.69 | kJ/mol | Joback Method |
| hfus | 53.94 | kJ/mol | Joback Method |
| hvap | 81.64 | kJ/mol | Joback Method |
| log10ws | -5.85 | | Crippen Method |
| logp | 5.484 | | Crippen Method |
| mcvol | 327.310 | ml/mol | McGowan Method |
| pc | 1044.62 | kPa | Joback Method |
| rinpol | 2394.00 | | NIST Webbook |
| rinpol | 2394.00 | | NIST Webbook |
| tb | 841.14 | K | Joback Method |
| tc | 1030.74 | K | Joback Method |
| tf | 486.46 | K | Joback Method |
| vc | 1.252 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1046.76 | J/mol×K | 841.14 | Joback Method |
| cpg | 1065.10 | J/mol×K | 872.74 | Joback Method |
| cpg | 1082.30 | J/mol×K | 904.34 | Joback Method |
| cpg | 1098.41 | J/mol×K | 935.94 | Joback Method |
| cpg | 1113.46 | J/mol×K | 967.54 | Joback Method |
| cpg | 1127.47 | J/mol×K | 999.14 | Joback Method |
| cpg | 1140.47 | J/mol×K | 1030.74 | 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=U392737&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 |