# DL-Alanine, N-methyl-N-(2-ethylhexyloxycarbonyl)-, 2-ethylhexyl ester

**Inchi:** InChI=1S/C21H41NO4/c1-7-11-13-18(9-3)15-25-20(23)17(5)22(6)21(24)26-16-19(10-4)14-12-

**InchiKey:** UMRRJBKAQLMSSH-UHFFFAOYSA-N

**Formula:** C21H41NO4

**SMILES:** CCCCC(CC)COC(=O)C(C)N(C)C(=O)OCC(CC)CCCC

**Mol. weight [g/mol]:** 371.55

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -238.44 | kJ/mol | Joback Method |
| hf | -914.68 | kJ/mol | Joback Method |
| hfus | 48.17 | kJ/mol | Joback Method |
| hvap | 81.53 | kJ/mol | Joback Method |
| log10ws | -5.51 | | Crippen Method |
| logp | 5.419 | | Crippen Method |
| mcvol | 331.610 | ml/mol | McGowan Method |
| pc | 1027.28 | kPa | Joback Method |
| rinpol | 2243.00 | | NIST Webbook |
| rinpol | 2243.00 | | NIST Webbook |
| tb | 843.58 | K | Joback Method |
| tc | 1034.17 | K | Joback Method |
| tf | 458.22 | K | Joback Method |
| vc | 1.260 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1075.42 | J/mol×K | 843.58 | Joback Method |
| cpg | 1094.38 | J/mol×K | 875.35 | Joback Method |
| cpg | 1112.13 | J/mol×K | 907.11 | Joback Method |
| cpg | 1128.71 | J/mol×K | 938.88 | Joback Method |
| cpg | 1144.15 | J/mol×K | 970.64 | Joback Method |
| cpg | 1158.47 | J/mol×K | 1002.41 | Joback Method |
| cpg | 1171.70 | J/mol×K | 1034.17 | Joback Method |

# Sources

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|---|---|
| **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=U392670&Units=SI |

# Legend

| | |
|---|---|
| **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 |