# DL-Alanine, N-methyl-N-hexyloxycarbonyl-, octadecyl ester

**Inchi:** InChI=1S/C29H57NO4/c1-5-7-9-11-12-13-14-15-16-17-18-19-20-21-22-24-25-33-28(31)2

**InchiKey:** URGKDINXBVFYKJ-UHFFFAOYSA-N

**Formula:** C29H57NO4

**SMILES:** CCCCCCCCCCCCCCCCCCOC(=O)C(C)N(C)C(=O)OCCCCCC

**Mol. weight [g/mol]:** 483.77

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -166.20 | kJ/mol | Joback Method |
| hf | -1069.24 | kJ/mol | Joback Method |
| hfus | 75.94 | kJ/mol | Joback Method |
| hvap | 100.12 | kJ/mol | Joback Method |
| log10ws | -9.35 | | Crippen Method |
| logp | 8.828 | | Crippen Method |
| mcvol | 444.330 | ml/mol | McGowan Method |
| pc | 656.12 | kPa | Joback Method |
| rinpol | 3184.00 | | NIST Webbook |
| rinpol | 3184.00 | | NIST Webbook |
| tb | 1027.50 | K | Joback Method |
| tc | 1285.62 | K | Joback Method |
| tf | 578.38 | K | Joback Method |
| vc | 1.720 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1585.48 | J/mol×K | 1027.50 | Joback Method |
| cpg | 1609.16 | J/mol×K | 1070.52 | Joback Method |
| cpg | 1630.51 | J/mol×K | 1113.54 | Joback Method |
| cpg | 1649.64 | J/mol×K | 1156.56 | Joback Method |
| cpg | 1666.68 | J/mol×K | 1199.58 | Joback Method |
| cpg | 1681.73 | J/mol×K | 1242.60 | Joback Method |
| cpg | 1694.92 | J/mol×K | 1285.62 | 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=U392647&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 |