# L-Leucine, N-methyl-N-(hexyloxycarbonyl)-, octadecyl ester

**Inchi:** InChI=1S/C32H63NO4/c1-6-8-10-12-13-14-15-16-17-18-19-20-21-22-23-25-26-36-31(34

**InchiKey:** KMINJWHDXNPOQF-SSEXGKCCSA-N

**Formula:** C32H63NO4

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

**Mol. weight [g/mol]:** 525.85

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -143.38 | kJ/mol | Joback Method |
| hf | -1136.44 | kJ/mol | Joback Method |
| hfus | 80.19 | kJ/mol | Joback Method |
| hvap | 106.41 | kJ/mol | Joback Method |
| log10ws | -10.36 | | Crippen Method |
| logp | 9.854 | | Crippen Method |
| mcvol | 486.600 | ml/mol | McGowan Method |
| pc | 571.24 | kPa | Joback Method |
| rinpol | 3301.00 | | NIST Webbook |
| rinpol | 3301.00 | | NIST Webbook |
| tb | 1095.70 | K | Joback Method |
| tc | 1398.14 | K | Joback Method |
| tf | 597.19 | K | Joback Method |
| vc | 1.881 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1782.81 | J/mol×K | 1095.70 | Joback Method |
| cpg | 1808.62 | J/mol×K | 1146.11 | Joback Method |
| cpg | 1831.28 | J/mol×K | 1196.51 | Joback Method |
| cpg | 1851.00 | J/mol×K | 1246.92 | Joback Method |
| cpg | 1868.01 | J/mol×K | 1297.33 | Joback Method |
| cpg | 1882.51 | J/mol×K | 1347.74 | Joback Method |
| cpg | 1894.71 | J/mol×K | 1398.14 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392356&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |