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

**Inchi:** InChI=1S/C30H59NO4/c1-6-8-10-12-13-14-15-16-17-18-19-20-21-23-24-34-29(32)28(26

**InchiKey:** RXROVURRSRBFDY-MUUNZHRXSA-N

**Formula:** C30H59NO4

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

**Mol. weight [g/mol]:** 497.79

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -160.22 | kJ/mol | Joback Method |
| hf | -1095.16 | kJ/mol | Joback Method |
| hfus | 75.00 | kJ/mol | Joback Method |
| hvap | 101.95 | kJ/mol | Joback Method |
| log10ws | -9.52 | | Crippen Method |
| logp | 9.074 | | Crippen Method |
| mcvol | 458.420 | ml/mol | McGowan Method |
| pc | 627.51 | kPa | Joback Method |
| rinpol | 3099.00 | | NIST Webbook |
| rinpol | 3099.00 | | NIST Webbook |
| tb | 1049.94 | K | Joback Method |
| tc | 1319.00 | K | Joback Method |
| tf | 574.65 | K | Joback Method |
| vc | 1.770 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1651.20 | J/mol×K | 1049.94 | Joback Method |
| cpg | 1675.29 | J/mol×K | 1094.78 | Joback Method |
| cpg | 1696.85 | J/mol×K | 1139.63 | Joback Method |
| cpg | 1716.00 | J/mol×K | 1184.47 | Joback Method |
| cpg | 1732.89 | J/mol×K | 1229.31 | Joback Method |
| cpg | 1747.65 | J/mol×K | 1274.16 | Joback Method |
| cpg | 1760.41 | J/mol×K | 1319.00 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392354&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 |