# l-Leucine, N-neopentyloxycarbonyl-N-methyl-, hexyl ester

**Inchi:** InChI=1S/C19H37NO4/c1-8-9-10-11-12-23-17(21)16(13-15(2)3)20(7)18(22)24-14-19(4,5

**InchiKey:** RIJMSNAZBLHAIO-UHFFFAOYSA-N

**Formula:** C19H37NO4

**SMILES:** CCCCCCOC(=O)C(CC(C)C)N(C)C(=O)OCC(C)(C)C

**Mol. weight [g/mol]:** 343.50

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -250.00 | kJ/mol | Joback Method |
| hf | -876.87 | kJ/mol | Joback Method |
| hfus | 39.10 | kJ/mol | Joback Method |
| hvap | 76.17 | kJ/mol | Joback Method |
| log10ws | -4.68 | | Crippen Method |
| logp | 4.639 | | Crippen Method |
| mcvol | 303.430 | ml/mol | McGowan Method |
| pc | 1175.24 | kPa | Joback Method |
| rinpol | 2006.00 | | NIST Webbook |
| tb | 795.03 | K | Joback Method |
| tc | 982.13 | K | Joback Method |
| tf | 453.10 | K | Joback Method |
| vc | 1.143 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 953.99 | J/mol×K | 795.03 | Joback Method |
| cpg | 972.25 | J/mol×K | 826.21 | Joback Method |
| cpg | 989.43 | J/mol×K | 857.40 | Joback Method |
| cpg | 1005.55 | J/mol×K | 888.58 | Joback Method |
| cpg | 1020.67 | J/mol×K | 919.76 | Joback Method |
| cpg | 1034.81 | J/mol×K | 950.95 | Joback Method |
| cpg | 1048.01 | J/mol×K | 982.13 | Joback Method |

# Sources

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|---|---|
| **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=U321910&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |