# L-Leucine, N-ethoxycarbonyl-N-methyl-, isobutyl ester

**Inchi:** InChI=1S/C14H27NO4/c1-7-18-14(17)15(6)12(8-10(2)3)13(16)19-9-11(4)5/h10-12H,7-9H

**InchiKey:** IEBCWZJJTRIGJR-UHFFFAOYSA-N

**Formula:** C14H27NO4

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

**Mol. weight [g/mol]:** 273.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -937.28 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 30.04 | kJ/mol | Joback Method |
| hvap | 78.75 | kJ/mol | Cheméo Relay (1.0) |
| ie | 8.74 | eV | Cheméo Relay (1.0) |
| logp | 2.689 | | Crippen Method |
| mcvol | 232.980 | ml/mol | McGowan Method |
| pc | 1668.70 | kPa | Joback Method |
| rinpol | 1614.00 | | NIST Webbook |
| tb | 560.91 | K | Cheméo Relay (1.0) |
| tc | 718.07 | K | Cheméo Relay (1.0) |
| tf | 252.62 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 663.68 | J/mol×K | 683.42 | Joback Method |
| cpg | 680.30 | J/mol×K | 713.80 | Joback Method |
| cpg | 696.07 | J/mol×K | 744.19 | Joback Method |
| cpg | 710.99 | J/mol×K | 774.57 | Joback Method |
| cpg | 725.07 | J/mol×K | 804.96 | Joback Method |
| cpg | 738.33 | J/mol×K | 835.34 | Joback Method |
| cpg | 750.77 | J/mol×K | 865.73 | Joback Method |

# Sources

| | |
|---|---|
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321921&Units=SI |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Cheméo Relay (1.0):** | |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **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 |