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

**Inchi:** InChI=1S/C21H41NO4/c1-6-8-9-10-11-12-13-14-15-16-26-20(23)19(17-18(3)4)22(5)21(2

**InchiKey:** IIEFYFJXUPPNIO-UHFFFAOYSA-N

**Formula:** C21H41NO4

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

**Mol. weight [g/mol]:** 371.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| hf | -1055.81 | kJ/mol | Cheméo Relay (1.0) |
| hfus | 51.69 | kJ/mol | Joback Method |
| hvap | 105.98 | kJ/mol | Cheméo Relay (1.0) |
| log10ws | -5.22 | | Cheméo Relay (1.0) |
| logp | 5.563 | | Crippen Method |
| mcvol | 331.610 | ml/mol | McGowan Method |
| rinpol | 2324.00 | | NIST Webbook |
| tb | 618.70 | K | Cheméo Relay (1.0) |
| tf | 267.80 | K | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1074.95 | J/mol×K | 844.02 | Joback Method |
| cpg | 1093.87 | J/mol×K | 875.71 | Joback Method |
| cpg | 1111.61 | J/mol×K | 907.40 | Joback Method |
| cpg | 1128.18 | J/mol×K | 939.09 | Joback Method |
| cpg | 1143.62 | J/mol×K | 970.78 | Joback Method |
| cpg | 1157.96 | J/mol×K | 1002.48 | Joback Method |
| cpg | 1171.23 | J/mol×K | 1034.17 | Joback Method |

## Sources

| | |
|---|---|
| **Cheméo Relay (1.0):** | |
| **Cheméo Relay (1.0, beta):** | |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321926&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 |

# Legend

| | |
|---|---|
| **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 |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tf:** | Normal melting (fusion) point |