# l-Leucine, N-ethoxycarbonyl-N-methyl-, pentadecyl ester

**Inchi:** InChI=1S/C25H49NO4/c1-6-8-9-10-11-12-13-14-15-16-17-18-19-20-30-24(27)23(21-22(3

**InchiKey:** FWZCAARLHWGSOM-UHFFFAOYSA-N

**Formula:** C25H49NO4

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

**Mol. weight [g/mol]:** 427.66

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -202.32 | kJ/mol | Joback Method |
| hf | -991.96 | kJ/mol | Joback Method |
| hfus | 62.05 | kJ/mol | Joback Method |
| hvap | 90.82 | kJ/mol | Joback Method |
| log10ws | -7.43 | | Crippen Method |
| logp | 7.124 | | Crippen Method |
| mcvol | 387.970 | ml/mol | McGowan Method |
| pc | 810.76 | kPa | Joback Method |
| rinpol | 2725.00 | | NIST Webbook |
| tb | 935.54 | K | Joback Method |
| tc | 1148.84 | K | Joback Method |
| tf | 518.30 | K | Joback Method |
| vc | 1.490 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1326.77 | J/mol×K | 935.54 | Joback Method |
| cpg | 1347.53 | J/mol×K | 971.09 | Joback Method |
| cpg | 1366.71 | J/mol×K | 1006.64 | Joback Method |
| cpg | 1384.35 | J/mol×K | 1042.19 | Joback Method |
| cpg | 1400.51 | J/mol×K | 1077.74 | Joback Method |
| cpg | 1415.24 | J/mol×K | 1113.29 | Joback Method |
| cpg | 1428.60 | J/mol×K | 1148.84 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U321929&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |