# l-Leucine, N-benzyloxycarbonyl-N-methyl-, isobutyl ester

**Inchi:** InChI=1S/C19H29NO4/c1-14(2)11-17(18(21)23-12-15(3)4)20(5)19(22)24-13-16-9-7-6-8-
**InchiKey:** DGKZHIXHVKODBP-UHFFFAOYSA-N
**Formula:** C19H29NO4
**SMILES:** CC(C)COC(=O)C(CC(C)C)N(C)C(=O)OCc1ccccc1
**Mol. weight [g/mol]:** 335.44

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -142.87 | kJ/mol | Joback Method |
| hf | -636.87 | kJ/mol | Joback Method |
| hfus | 37.03 | kJ/mol | Joback Method |
| hvap | 79.36 | kJ/mol | Joback Method |
| log10ws | -4.28 | | Crippen Method |
| logp | 3.869 | | Crippen Method |
| mcvol | 279.670 | ml/mol | McGowan Method |
| pc | 1482.71 | kPa | Joback Method |
| rinpol | 2157.00 | | NIST Webbook |
| rinpol | 2157.00 | | NIST Webbook |
| tb | 824.50 | K | Joback Method |
| tc | 1028.88 | K | Joback Method |
| tf | 462.10 | K | Joback Method |
| vc | 1.040 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 863.34 | J/mol×K | 824.50 | Joback Method |
| cpg | 879.82 | J/mol×K | 858.56 | Joback Method |
| cpg | 895.09 | J/mol×K | 892.63 | Joback Method |
| cpg | 909.19 | J/mol×K | 926.69 | Joback Method |
| cpg | 922.15 | J/mol×K | 960.75 | Joback Method |
| cpg | 934.00 | J/mol×K | 994.82 | Joback Method |
| cpg | 944.79 | J/mol×K | 1028.88 | 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=U322036&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 |