# l-Phenylalanine, N-caproyl-, methyl ester

**Inchi:** InChI=1S/C16H23NO3/c1-3-4-6-11-15(18)17-14(16(19)20-2)12-13-9-7-5-8-10-13/h5,7-10
**InchiKey:** IZQJDSLVCFGOEO-UHFFFAOYSA-N
**Formula:** C16H23NO3
**SMILES:** CCCCCC(=O)NC(Cc1ccccc1)C(=O)OC
**Mol. weight [g/mol]:** 277.36

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -79.64 | kJ/mol | Joback Method |
| hf | -446.23 | kJ/mol | Joback Method |
| hfus | 37.20 | kJ/mol | Joback Method |
| hvap | 75.44 | kJ/mol | Joback Method |
| log10ws | -3.56 | | Crippen Method |
| logp | 2.467 | | Crippen Method |
| mcvol | 231.530 | ml/mol | McGowan Method |
| pc | 1901.92 | kPa | Joback Method |
| rinpol | 2023.00 | | NIST Webbook |
| rinpol | 2023.00 | | NIST Webbook |
| tb | 772.05 | K | Joback Method |
| tc | 978.12 | K | Joback Method |
| tf | 456.25 | K | Joback Method |
| vc | 0.882 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 678.31 | J/mol×K | 772.05 | Joback Method |
| cpg | 693.41 | J/mol×K | 806.40 | Joback Method |
| cpg | 707.49 | J/mol×K | 840.74 | Joback Method |
| cpg | 720.56 | J/mol×K | 875.09 | Joback Method |
| cpg | 732.67 | J/mol×K | 909.43 | Joback Method |
| cpg | 743.85 | J/mol×K | 943.78 | Joback Method |
| cpg | 754.13 | J/mol×K | 978.12 | 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=U299737&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 |