# Butyl p-butylaminobenzoate

**Inchi:** InChI=1S/C15H23NO2/c1-3-5-11-16-14-9-7-13(8-10-14)15(17)18-12-6-4-2/h7-10,16H,3-
**InchiKey:** KRNUEIBLNHKQGZ-UHFFFAOYSA-N
**Formula:** C15H23NO2
**SMILES:** CCCCNc1ccc(C(=O)OCCCC)cc1
**Mol. weight [g/mol]:** 249.35

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 33.67 | kJ/mol | Joback Method |
| hf | -319.20 | kJ/mol | Joback Method |
| hfus | 36.14 | kJ/mol | Joback Method |
| hvap | 67.51 | kJ/mol | Joback Method |
| log10ws | -4.23 | | Crippen Method |
| logp | 3.855 | | Crippen Method |
| mcvol | 215.870 | ml/mol | McGowan Method |
| pc | 1918.62 | kPa | Joback Method |
| rinpol | 2344.00 | | NIST Webbook |
| rinpol | 2344.00 | | NIST Webbook |
| rinpol | 2359.00 | | NIST Webbook |
| rinpol | 2374.00 | | NIST Webbook |
| tb | 700.72 | K | Joback Method |
| tc | 899.86 | K | Joback Method |
| tf | 422.57 | K | Joback Method |
| vc | 0.827 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 602.88 | J/mol×K | 700.72 | Joback Method |
| cpg | 618.93 | J/mol×K | 733.91 | Joback Method |
| cpg | 634.05 | J/mol×K | 767.10 | Joback Method |
| cpg | 648.26 | J/mol×K | 800.29 | Joback Method |
| cpg | 661.58 | J/mol×K | 833.48 | Joback Method |
| cpg | 674.06 | J/mol×K | 866.67 | Joback Method |

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|---|---|---|---|---|
| cpg | 685.70 | J/mol×K | 899.86 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R578811&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |