# Benzoic acid, 4-tert-butyl-, butyl ester

**Other names:** Butyl 4-tert-butylbenzoate
**Inchi:** InChI=1S/C15H22O2/c1-5-6-11-17-14(16)12-7-9-13(10-8-12)15(2,3)4/h7-10H,5-6,11H2,1
**InchiKey:** BMSNGGLCKZGIEY-UHFFFAOYSA-N
**Formula:** C15H22O2
**SMILES:** CCCCOC(=O)c1ccc(C(C)(C)C)cc1
**Mol. weight [g/mol]:** 234.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -52.88 | kJ/mol | Joback Method |
| hf | -381.42 | kJ/mol | Joback Method |
| hfus | 23.63 | kJ/mol | Joback Method |
| hvap | 59.78 | kJ/mol | Joback Method |
| log10ws | -4.28 | | Crippen Method |
| logp | 3.941 | | Crippen Method |
| mcvol | 205.890 | ml/mol | McGowan Method |
| pc | 1928.74 | kPa | Joback Method |
| rinpol | 1689.00 | | NIST Webbook |
| rinpol | 1748.00 | | NIST Webbook |
| tb | 647.32 | K | Joback Method |
| tc | 856.19 | K | Joback Method |
| tf | 372.33 | K | Joback Method |
| vc | 0.780 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 548.94 | J/mol×K | 647.32 | Joback Method |
| cpg | 625.24 | J/mol×K | 821.38 | Joback Method |
| cpg | 611.93 | J/mol×K | 786.57 | Joback Method |
| cpg | 597.69 | J/mol×K | 751.76 | Joback Method |
| cpg | 582.47 | J/mol×K | 716.94 | Joback Method |
| cpg | 566.24 | J/mol×K | 682.13 | Joback Method |
| cpg | 637.67 | J/mol×K | 856.19 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001166 | Pa×s | 647.32 | Joback Method |
| dvisc | 0.0001531 | Pa×s | 601.49 | Joback Method |
| dvisc | 0.0002103 | Pa×s | 555.66 | Joback Method |
| dvisc | 0.0003057 | Pa×s | 509.82 | Joback Method |
| dvisc | 0.0004787 | Pa×s | 463.99 | Joback Method |
| dvisc | 0.0008268 | Pa×s | 418.16 | Joback Method |
| dvisc | 0.0016339 | Pa×s | 372.33 | Joback Method |

# Sources

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|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U406140&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |