# 4-Butylbenzoic acid, 4-biphenyl ester

**Inchi:** InChI=1S/C23H22O2/c1-2-3-7-18-10-12-21(13-11-18)23(24)25-22-16-14-20(15-17-22)19
**InchiKey:** LPTPHOTZYYIPFH-UHFFFAOYSA-N
**Formula:** C23H22O2
**SMILES:** CCCCc1ccc(C(=O)Oc2ccc(-c3ccccc3)cc2)cc1
**Mol. weight [g/mol]:** 330.42

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 226.83 | kJ/mol | Joback Method |
| hf | -76.20 | kJ/mol | Joback Method |
| hfus | 39.46 | kJ/mol | Joback Method |
| hvap | 84.10 | kJ/mol | Joback Method |
| log10ws | -7.80 | | Crippen Method |
| logp | 5.915 | | Crippen Method |
| mcvol | 271.090 | ml/mol | McGowan Method |
| pc | 1711.78 | kPa | Joback Method |
| rinpol | 3113.00 | | NIST Webbook |
| tb | 891.93 | K | Joback Method |
| tc | 1136.45 | K | Joback Method |
| tf | 525.43 | K | Joback Method |
| vc | 1.024 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 814.24 | J/mol×K | 891.93 | Joback Method |
| cpg | 829.55 | J/mol×K | 932.68 | Joback Method |
| cpg | 843.45 | J/mol×K | 973.44 | Joback Method |
| cpg | 856.01 | J/mol×K | 1014.19 | Joback Method |
| cpg | 867.35 | J/mol×K | 1054.95 | Joback Method |
| cpg | 877.54 | J/mol×K | 1095.70 | Joback Method |
| cpg | 886.68 | J/mol×K | 1136.45 | Joback Method |
| dvisc | 0.0004953 | Pa×s | 525.43 | Joback Method |
| dvisc | 0.0002819 | Pa×s | 586.51 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0001785 | Pa×s | 647.60 | Joback Method |
| dvisc | 0.0001223 | Pa×s | 708.68 | Joback Method |
| dvisc | 0.0000890 | Pa×s | 769.76 | Joback Method |
| dvisc | 0.0000678 | Pa×s | 830.85 | Joback Method |
| dvisc | 0.0000536 | Pa×s | 891.93 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354325&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

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