# Benzanilide, n,4-di-tert-butyl-

**Inchi:** InChI=1S/C21H27NO/c1-20(2,3)17-12-14-18(15-13-17)22(21(4,5)6)19(23)16-10-8-7-9-11
**InchiKey:** UPVMUZDIHKYDAL-UHFFFAOYSA-N
**Formula:** C21H27NO
**SMILES:** CC(C)(C)c1ccc(N(C(=O)c2ccccc2)C(C)(C)C)cc1
**Mol. weight [g/mol]:** 309.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 328.67 | kJ/mol | Joback Method |
| hf | -77.73 | kJ/mol | Joback Method |
| hfus | 27.63 | kJ/mol | Joback Method |
| hvap | 73.75 | kJ/mol | Joback Method |
| log10ws | -6.03 | | Crippen Method |
| logp | 5.429 | | Crippen Method |
| mcvol | 270.780 | ml/mol | McGowan Method |
| pc | 1615.47 | kPa | Joback Method |
| tb | 798.07 | K | Joback Method |
| tc | 1034.47 | K | Joback Method |
| tf | 479.03 | K | Joback Method |
| vc | 0.998 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 811.16 | J/mol×K | 798.07 | Joback Method |
| cpg | 829.61 | J/mol×K | 837.47 | Joback Method |
| cpg | 846.66 | J/mol×K | 876.87 | Joback Method |
| cpg | 862.46 | J/mol×K | 916.27 | Joback Method |
| cpg | 877.18 | J/mol×K | 955.67 | Joback Method |
| cpg | 890.96 | J/mol×K | 995.07 | Joback Method |
| cpg | 903.98 | J/mol×K | 1034.47 | Joback Method |

# Sources

| | |
|---|---|
| **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=B6009282&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |