# Phenol, 2,4-di-t-butyl-6-nitro-

**Inchi:** InChI=1S/C14H21NO3/c1-13(2,3)9-7-10(14(4,5)6)12(16)11(8-9)15(17)18/h7-8,16H,1-6H
**InchiKey:** GVKJWGRAPDVEMC-UHFFFAOYSA-N
**Formula:** C14H21NO3
**SMILES:** CC(C)(C)c1cc([N+](=O)[O-])c(O)c(C(C)(C)C)c1
**Mol. weight [g/mol]:** 251.32
**CAS:** 20039-94-5

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 46.76 | kJ/mol | Joback Method |
| hf | -324.27 | kJ/mol | Joback Method |
| hfus | 27.60 | kJ/mol | Joback Method |
| hvap | 77.37 | kJ/mol | Joback Method |
| log10ws | -4.30 | | Crippen Method |
| logp | 3.895 | | Crippen Method |
| mcvol | 207.650 | ml/mol | McGowan Method |
| pc | 2351.92 | kPa | Joback Method |
| tb | 782.36 | K | Joback Method |
| tc | 1032.60 | K | Joback Method |
| tf | 559.17 | K | Joback Method |
| vc | 0.738 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 617.81 | J/mol×K | 782.36 | Joback Method |
| cpg | 632.82 | J/mol×K | 824.07 | Joback Method |
| cpg | 646.95 | J/mol×K | 865.77 | Joback Method |
| cpg | 660.38 | J/mol×K | 907.48 | Joback Method |
| cpg | 673.28 | J/mol×K | 949.19 | Joback Method |
| cpg | 685.86 | J/mol×K | 990.89 | Joback Method |
| cpg | 698.29 | J/mol×K | 1032.60 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C20039945&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

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