

# 1,1'-Biphenyl-3-ol, 3'-chloro

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C12H9ClO/c13-11-5-1-3-9(7-11)10-4-2-6-12(14)8-10/h1-8,14H |
| <b>InchiKey:</b>            | FRQIKHFDYHKAHE-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C12H9ClO   |
| <b>SMILES:</b>              | Oc1cccc(-c2cccc(Cl)c2)c1   |
| <b>Mol. weight [g/mol]:</b> | 204.65   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 98.80   | kJ/mol               | Joback Method  |
| hf            | -22.47  | kJ/mol               | Joback Method  |
| hfus          | 24.51   | kJ/mol               | Joback Method  |
| hvap          | 64.92   | kJ/mol               | Joback Method  |
| log10ws       | -4.31   |                      | Crippen Method |
| logp          | 3.713   |                      | Crippen Method |
| mcvol         | 150.530 | ml/mol               | McGowan Method |
| pc            | 3853.09 | kPa                  | Joback Method  |
| rinpol        | 1849.00 |                      | NIST Webbook   |
| rinpol        | 1849.00 |                      | NIST Webbook   |
| tb            | 650.35  | K                    | Joback Method  |
| tc            | 914.63  | K                    | Joback Method  |
| tf            | 432.00  | K                    | Joback Method  |
| vc            | 0.506   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 351.29    | J/molxK | 650.35          | Joback Method |
| cpg           | 363.75    | J/molxK | 694.40          | Joback Method |
| cpg           | 375.13    | J/molxK | 738.44          | Joback Method |
| cpg           | 385.60    | J/molxK | 782.49          | Joback Method |
| cpg           | 395.30    | J/molxK | 826.54          | Joback Method |
| cpg           | 404.39    | J/molxK | 870.58          | Joback Method |
| cpg           | 413.02    | J/molxK | 914.63          | Joback Method |
| dvisc         | 0.0006154 | Paxs    | 432.00          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002923 | Paxs | 468.39 | Joback Method |
| dvisc | 0.0001545 | Paxs | 504.78 | Joback Method |
| dvisc | 0.0000890 | Paxs | 541.17 | Joback Method |
| dvisc | 0.0000550 | Paxs | 577.57 | Joback Method |
| dvisc | 0.0000359 | Paxs | 613.96 | Joback Method |
| dvisc | 0.0000246 | Paxs | 650.35 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R343690&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R343690&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>rinpol:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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