

# 1,1'-Biphenyl-3-ol, 3',4-dichloro

|                             |   |
|-----------------------------|---|
| <b>Inchi:</b>               | InChI=1S/C12H8Cl2O/c13-10-3-1-2-8(6-10)9-4-5-11(14)12(15)7-9/h1-7,15H |
| <b>InchiKey:</b>            | WGSVCHKOTNOIFO-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H8Cl2O   |
| <b>SMILES:</b>              | Oc1cc(-c2cccc(Cl)c2)ccc1Cl  |
| <b>Mol. weight [g/mol]:</b> | 239.10  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 77.24   | kJ/mol               | Joback Method  |
| hf            | -49.68  | kJ/mol               | Joback Method  |
| hfus          | 28.32   | kJ/mol               | Joback Method  |
| hvap          | 69.97   | kJ/mol               | Joback Method  |
| log10ws       | -4.99   |                      | Crippen Method |
| logp          | 4.366   |                      | Crippen Method |
| mcvol         | 162.770 | ml/mol               | McGowan Method |
| pc            | 3615.89 | kPa                  | Joback Method  |
| rinpol        | 1939.00 |                      | NIST Webbook   |
| tb            | 692.76  | K                    | Joback Method  |
| tc            | 960.07  | K                    | Joback Method  |
| tf            | 474.44  | K                    | Joback Method  |
| vc            | 0.555   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 371.08    | J/molxK | 692.76          | Joback Method |
| cpg           | 419.03    | J/molxK | 915.52          | Joback Method |
| cpg           | 410.63    | J/molxK | 870.97          | Joback Method |
| cpg           | 401.79    | J/molxK | 826.42          | Joback Method |
| cpg           | 392.36    | J/molxK | 781.86          | Joback Method |
| cpg           | 382.17    | J/molxK | 737.31          | Joback Method |
| cpg           | 427.12    | J/molxK | 960.07          | Joback Method |
| dvisc         | 0.0000190 | Paxs    | 692.76          | Joback Method |
| dvisc         | 0.0000267 | Paxs    | 656.37          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000391 | Paxs | 619.99 | Joback Method |
| dvisc | 0.0000600 | Paxs | 583.60 | Joback Method |
| dvisc | 0.0000975 | Paxs | 547.21 | Joback Method |
| dvisc | 0.0001697 | Paxs | 510.83 | Joback Method |
| dvisc | 0.0003217 | Paxs | 474.44 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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=R343645&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R343645&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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