

[1,1'-Biphenyl]-4-ol, 3,4'-dichloro-

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|-----------------------------|---|
| Other names: | 3,4'-Dichloro-4-biphenylol |
| Inchi: | InChI=1S/C12H8Cl2O/c13-10-4-1-8(2-5-10)9-3-6-12(15)11(14)7-9/h1-7,15H |
| InchiKey: | UHKLHHYQCUBQDI-UHFFFAOYSA-N |
| Formula: | C12H8Cl2O |
| SMILES: | Oc1ccc(-c2ccc(Cl)cc2)cc1Cl |
| Mol. weight [g/mol]: | 239.10 |
| CAS: | 53905-31-0 |

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 | 1950.00 | | NIST Webbook |
| tb | 692.76 | K | Joback Method |
| tc | 960.07 | K | Joback Method |
| tf | 474.44 | K | Joback Method |
| vc | 0.555 | m3/kmol | Joback Method |

Temperature Dependent Properties

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

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003217 | Paxs | 474.44 | Joback Method |
| dvisc | 0.0001697 | Paxs | 510.83 | Joback Method |
| dvisc | 0.0000975 | Paxs | 547.21 | Joback Method |
| dvisc | 0.0000600 | Paxs | 583.60 | Joback Method |
| dvisc | 0.0000391 | Paxs | 619.99 | Joback Method |
| dvisc | 0.0000267 | Paxs | 656.37 | Joback Method |
| dvisc | 0.0000190 | Paxs | 692.76 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C53905310&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| 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 |
| mvol: | 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 |

Latest version available from:

<https://www.chemeo.com/cid/14-575-8/1-1-Biphenyl-4-ol-3-4-dichloro.pdf>

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