

[1,1'-Biphenyl]-2,4'-diol

| | |
|-----------------------------|---|
| Inchi: | InChI=1S/C12H10O2/c13-10-7-5-9(6-8-10)11-3-1-2-4-12(11)14/h1-8,13-14H |
| InchiKey: | JHOPNNTTBHXSHY-UHFFFAOYSA-N |
| Formula: | C12H10O2 |
| SMILES: | Oc1ccc(-c2ccccc2O)cc1 |
| Mol. weight [g/mol]: | 186.21 |
| CAS: | 611-62-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -34.26 | kJ/mol | Joback Method |
| hf | -172.57 | kJ/mol | Joback Method |
| hfus | 26.48 | kJ/mol | Joback Method |
| hvap | 72.89 | kJ/mol | Joback Method |
| log10ws | -3.17 | | Crippen Method |
| logp | 2.765 | | Crippen Method |
| mcvol | 144.160 | ml/mol | McGowan Method |
| pc | 5029.93 | kPa | Joback Method |
| rinpol | 1820.00 | | NIST Webbook |
| rinpol | 1820.00 | | NIST Webbook |
| tb | 688.56 | K | Joback Method |
| tc | 956.80 | K | Joback Method |
| tf | 501.28 | K | Joback Method |
| vc | 0.423 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 373.78 | J/molxK | 688.56 | Joback Method |
| cpg | 426.49 | J/molxK | 912.09 | Joback Method |
| cpg | 416.72 | J/molxK | 867.39 | Joback Method |
| cpg | 406.80 | J/molxK | 822.68 | Joback Method |
| cpg | 396.50 | J/molxK | 777.97 | Joback Method |
| cpg | 385.57 | J/molxK | 733.27 | Joback Method |
| cpg | 436.36 | J/molxK | 956.80 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000021 | Paxs | 688.56 | Joback Method |
| dvisc | 0.0000033 | Paxs | 657.35 | Joback Method |
| dvisc | 0.0000054 | Paxs | 626.13 | Joback Method |
| dvisc | 0.0000093 | Paxs | 594.92 | Joback Method |
| dvisc | 0.0000170 | Paxs | 563.71 | Joback Method |
| dvisc | 0.0000335 | Paxs | 532.49 | Joback Method |
| dvisc | 0.0000720 | Paxs | 501.28 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 481.20 | K | 1.50 | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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 |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C611621&Units=SI |

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 |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |

tbrp: Boiling point at reduced pressure
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

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