

1,1'-Biphenyl-2-ol, 2',4,6-trichloro

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H7Cl3O/c13-7-5-10(15)12(11(16)6-7)8-3-1-2-4-9(8)14/h1-6,16H |
| InchiKey: | HXUKDKDGVVYEV-UHFFFAOYSA-N |
| Formula: | C12H7Cl3O |
| SMILES: | Oc1cc(Cl)cc(Cl)c1-c1ccccc1Cl |
| Mol. weight [g/mol]: | 273.54 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 55.68 | kJ/mol | Joback Method |
| hf | -76.89 | kJ/mol | Joback Method |
| hfus | 32.12 | kJ/mol | Joback Method |
| hvap | 75.01 | kJ/mol | Joback Method |
| log10ws | -5.68 | | Crippen Method |
| logp | 5.019 | | Crippen Method |
| mcvol | 175.010 | ml/mol | McGowan Method |
| pc | 3399.94 | kPa | Joback Method |
| rinpol | 1916.00 | | NIST Webbook |
| tb | 735.17 | K | Joback Method |
| tc | 1004.96 | K | Joback Method |
| tf | 516.88 | K | Joback Method |
| vc | 0.605 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 388.99 | J/mol×K | 735.17 | Joback Method |
| cpg | 432.62 | J/mol×K | 959.99 | Joback Method |
| cpg | 424.77 | J/mol×K | 915.03 | Joback Method |
| cpg | 416.63 | J/mol×K | 870.06 | Joback Method |
| cpg | 408.05 | J/mol×K | 825.10 | Joback Method |
| cpg | 398.89 | J/mol×K | 780.13 | Joback Method |
| cpg | 440.33 | J/mol×K | 1004.96 | Joback Method |
| dvisc | 0.0000147 | Paxs | 735.17 | Joback Method |
| dvisc | 0.0000200 | Paxs | 698.79 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0000283 | Paxs | 662.41 | Joback Method |
| dvisc | 0.0000415 | Paxs | 626.03 | Joback Method |
| dvisc | 0.0000639 | Paxs | 589.64 | Joback Method |
| dvisc | 0.0001042 | Paxs | 553.26 | Joback Method |
| dvisc | 0.0001819 | Paxs | 516.88 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=R343170&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| mccvol: | 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/15-918-6/1-1-Biphenyl-2-ol-2-4-6-trichloro.pdf>

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