

# 1,1'-Biphenyl-3-ol, 2',5',6-trichloro

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C12H7Cl3O/c13-7-1-3-11(14)9(5-7)10-6-8(16)2-4-12(10)15/h1-6,16H |
| <b>InchiKey:</b>            | DOWLEXFVSMYPPW-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C12H7Cl3O  |
| <b>SMILES:</b>              | Oc1ccc(Cl)c(-c2cc(Cl)ccc2Cl)c1   |
| <b>Mol. weight [g/mol]:</b> | 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        | 2047.00 |         | NIST Webbook   |
| rinpol        | 2047.00 |         | NIST Webbook   |
| tb            | 735.17  | K       | Joback Method  |
| tc            | 1004.96 | K       | Joback Method  |
| tf            | 516.88  | K       | Joback Method  |
| vc            | 0.605   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

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

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0000200 | Paxs | 698.79 | Joback Method |
| 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

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R343472&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R343472&amp;Units=SI</a> |
| <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>                     |

## Legend

|                            |   |
|----------------------------|---|
| <b>cp<sub>g</sub>:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>              | Dynamic viscosity                               |
| <b>g<sub>f</sub>:</b>      | Standard Gibbs free energy of formation         |
| <b>h<sub>f</sub>:</b>      | Enthalpy of formation at standard conditions    |
| <b>h<sub>fus</sub>:</b>    | Enthalpy of fusion at standard conditions       |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</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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