

# [1,1'-Biphenyl]-2-ol, 3,5-dichloro-

|                      |                                                                                                                                                                                                                              |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-Biphenylol, 3,5-dichloro-<br>2-Hydroxy-3,5-dichlorobiphenyl<br>2,4-Dichloro-6-phenylphenol<br>4,6-Dichloro-o-phenylphenol<br>3,5-Dichloro-(1,1'-biphenyl)-2-ol<br>3,5-Dichloro-2-biphenylol<br>4,6-Dichloro-2-phenylphenol |
| Inchi:               | InChI=1S/C12H8Cl2O/c13-9-6-10(12(15)11(14)7-9)8-4-2-1-3-5-8/h1-7,15H                                                                                                                                                         |
| InchiKey:            | AFXPPGXJWHJULD-UHFFFAOYSA-N                                                                                                                                                                                                  |
| Formula:             | C12H8Cl2O                                                                                                                                                                                                                    |
| SMILES:              | Oc1c(Cl)cc(Cl)cc1-c1ccccc1                                                                                                                                                                                                   |
| Mol. weight [g/mol]: | 239.10                                                                                                                                                                                                                       |
| CAS:                 | 5335-24-0                                                                                                                                                                                                                    |

## 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        | 1871.00 |         | 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/mol×K | 692.76          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 382.17    | J/mol×K | 737.31 | Joback Method |
| cpg   | 392.36    | J/mol×K | 781.86 | Joback Method |
| cpg   | 401.79    | J/mol×K | 826.42 | Joback Method |
| cpg   | 410.63    | J/mol×K | 870.97 | Joback Method |
| cpg   | 419.03    | J/mol×K | 915.52 | Joback Method |
| cpg   | 427.12    | J/mol×K | 960.07 | Joback Method |
| dvisc | 0.0003217 | Pa×s    | 474.44 | Joback Method |
| dvisc | 0.0001697 | Pa×s    | 510.83 | Joback Method |
| dvisc | 0.0000975 | Pa×s    | 547.21 | Joback Method |
| dvisc | 0.0000600 | Pa×s    | 583.60 | Joback Method |
| dvisc | 0.0000391 | Pa×s    | 619.99 | Joback Method |
| dvisc | 0.0000267 | Pa×s    | 656.37 | Joback Method |
| dvisc | 0.0000190 | Pa×s    | 692.76 | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C5335240&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5335240&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>                           |
| <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>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                   |

**vc:** Critical Volume

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