

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

|                      |                                                                                                                                                                                       |
|----------------------|---------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 1,4-dichloro-2-(3-chlorophenyl)benzene<br>2,3',5-PCB<br>2,3',5-Trichloro-1,1'-biphenyl<br>2,3',5-Trichlorobiphenyl<br>2,5,3'-Trichlorobiphenyl<br>3,2',5'-Trichlorobiphenyl<br>PCB 26 |
| Inchi:               | InChI=1S/C12H7Cl3/c13-9-3-1-2-8(6-9)11-7-10(14)4-5-12(11)15/h1-7H                                                                                                                     |
| InchiKey:            | ONNCPBRWFSKDMQ-UHFFFAOYSA-N                                                                                                                                                           |
| Formula:             | C12H7Cl3                                                                                                                                                                              |
| SMILES:              | Clc1cccc(-c2cc(Cl)ccc2Cl)c1                                                                                                                                                           |
| Mol. weight [g/mol]: | 257.54                                                                                                                                                                                |
| CAS:                 | 38444-81-4                                                                                                                                                                            |

## Physical Properties

| Property code | Value   | Unit   | Source                               |
|---------------|---------|--------|--------------------------------------|
| gf            | 210.30  | kJ/mol | Joback Method                        |
| hf            | 100.42  | kJ/mol | Joback Method                        |
| hfus          | 26.34   | kJ/mol | Joback Method                        |
| hvap          | 62.00   | kJ/mol | Joback Method                        |
| log10ws       | -6.01   |        | Estimated Solubility Method          |
| log10ws       | -6.01   |        | Aqueous Solubility Prediction Method |
| logp          | 5.314   |        | Crippen Method                       |
| mcvol         | 169.140 | ml/mol | McGowan Method                       |
| pc            | 2878.12 | kPa    | Joback Method                        |
| rinpol        | 1843.00 |        | NIST Webbook                         |
| rinpol        | 1836.00 |        | NIST Webbook                         |
| rinpol        | 1834.50 |        | NIST Webbook                         |
| rinpol        | 1844.10 |        | NIST Webbook                         |
| rinpol        | 1814.00 |        | NIST Webbook                         |
| rinpol        | 1846.00 |        | NIST Webbook                         |
| rinpol        | 1825.10 |        | NIST Webbook                         |
| rinpol        | 1843.00 |        | NIST Webbook                         |
| rinpol        | 1836.00 |        | NIST Webbook                         |
| rinpol        | 1843.00 |        | NIST Webbook                         |

|        |         |         |               |
|--------|---------|---------|---------------|
| rinpol | 1843.60 |         | NIST Webbook  |
| tb     | 654.55  | K       | Joback Method |
| tc     | 917.95  | K       | Joback Method |
| tf     | 405.16  | K       | Joback Method |
| vc     | 0.638   | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 349.20    | J/mol×K | 654.55          | Joback Method |
| cpg           | 360.92    | J/mol×K | 698.45          | Joback Method |
| cpg           | 371.61    | J/mol×K | 742.35          | Joback Method |
| cpg           | 381.33    | J/mol×K | 786.25          | Joback Method |
| cpg           | 390.14    | J/mol×K | 830.15          | Joback Method |
| cpg           | 398.13    | J/mol×K | 874.05          | Joback Method |
| cpg           | 405.36    | J/mol×K | 917.95          | Joback Method |
| dvisc         | 0.0010725 | Pa×s    | 405.16          | Joback Method |
| dvisc         | 0.0006985 | Pa×s    | 446.73          | Joback Method |
| dvisc         | 0.0004893 | Pa×s    | 488.29          | Joback Method |
| dvisc         | 0.0003625 | Pa×s    | 529.86          | Joback Method |
| dvisc         | 0.0002805 | Pa×s    | 571.42          | Joback Method |
| dvisc         | 0.0002248 | Pa×s    | 612.99          | Joback Method |
| dvisc         | 0.0001852 | Pa×s    | 654.55          | Joback Method |

## Sources

|                                              |                                                                                                                                                                                                                         |
|----------------------------------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>                         | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C38444814&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C38444814&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>Joback Method:</b>                        | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                                                   |
| <b>Aqueous Solubility Prediction Method:</b> | <a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a> |
| <b>Estimated Solubility Method:</b>          | <a href="http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt">http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt</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

**cpg:** 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                   |
| <b>vc:</b>      | Critical Volume                                 |

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