

# 1,1'-Biphenyl, 3,3'-bis-(1-methylethyl)

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | 3,3'-Diisopropylbiphenyl                                                         |
| Inchi:               | InChI=1S/C18H22/c1-13(2)15-7-5-9-17(11-15)18-10-6-8-16(12-18)14(3)4/h5-14H,1-4H3 |
| InchiKey:            | PYXYRWLLNHRLM-UHFFFAOYSA-N                                                       |
| Formula:             | C18H22                                                                           |
| SMILES:              | CC(C)c1cccc(-c2cccc(C(C)C)c2)c1                                                  |
| Mol. weight [g/mol]: | 238.37                                                                           |
| CAS:                 | 69375-12-8                                                                       |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 301.36  | kJ/mol  | Joback Method  |
| hf            | 24.71   | kJ/mol  | Joback Method  |
| hfus          | 22.63   | kJ/mol  | Joback Method  |
| hvap          | 60.76   | kJ/mol  | Joback Method  |
| log10ws       | -6.44   |         | Crippen Method |
| logp          | 5.600   |         | Crippen Method |
| mcvol         | 216.960 | ml/mol  | McGowan Method |
| pc            | 1893.65 | kPa     | Joback Method  |
| tb            | 673.68  | K       | Joback Method  |
| tc            | 905.93  | K       | Joback Method  |
| tf            | 340.50  | K       | Joback Method  |
| vc            | 0.816   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 578.18    | J/mol×K | 673.68          | Joback Method |
| cpg           | 663.54    | J/mol×K | 867.22          | Joback Method |
| cpg           | 648.92    | J/mol×K | 828.51          | Joback Method |
| cpg           | 633.14    | J/mol×K | 789.80          | Joback Method |
| cpg           | 616.14    | J/mol×K | 751.10          | Joback Method |
| cpg           | 597.85    | J/mol×K | 712.39          | Joback Method |
| cpg           | 677.08    | J/mol×K | 905.93          | Joback Method |
| dvisc         | 0.0001049 | Pa×s    | 673.68          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001378 | Pa×s | 618.15 | Joback Method |
| dvisc | 0.0001911 | Pa×s | 562.62 | Joback Method |
| dvisc | 0.0002845 | Pa×s | 507.09 | Joback Method |
| dvisc | 0.0004672 | Pa×s | 451.56 | Joback Method |
| dvisc | 0.0008817 | Pa×s | 396.03 | Joback Method |
| dvisc | 0.0020468 | Pa×s | 340.50 | Joback Method |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                         |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C69375128&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C69375128&amp;Units=SI</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>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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