

# 1,1'-Biphenyl, 2-fluoro-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 2-Fluoro-1,1'-biphenyl<br>2-Fluorobiphenyl<br>o-Fluorobiphenyl<br>2-Fluorodiphenyl<br>o-Fluorodiphenyl<br>Biphenyl, 2-fluoro- |
| <b>Inchi:</b>               | InChI=1S/C12H9F/c13-12-9-5-4-8-11(12)10-6-2-1-3-7-10/h1-9H  |
| <b>InchiKey:</b>            | KLECYOQFQXJYBC-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C12H9F  |
| <b>SMILES:</b>              | Fc1ccccc1-c1ccccc1  |
| <b>Mol. weight [g/mol]:</b> | 172.20  |
| <b>CAS:</b>                 | 321-60-8  |

## Physical Properties

| Property code | Value       | Unit                 | Source         |
|---------------|-------------|----------------------|----------------|
| gf            | 70.54       | kJ/mol               | Joback Method  |
| hf            | -25.53      | kJ/mol               | Joback Method  |
| hfus          | 17.61       | kJ/mol               | Joback Method  |
| hvap          | 46.70       | kJ/mol               | Joback Method  |
| ie            | 8.20 ± 0.02 | eV                   | NIST Webbook   |
| log10ws       | -4.41       |                      | Crippen Method |
| logp          | 3.493       |                      | Crippen Method |
| mcvol         | 134.190     | ml/mol               | McGowan Method |
| pc            | 3199.16     | kPa                  | Joback Method  |
| rinpola       | 232.03      |                      | NIST Webbook   |
| rinpola       | 233.50      |                      | NIST Webbook   |
| rinpola       | 231.69      |                      | NIST Webbook   |
| rinpola       | 1346.00     |                      | NIST Webbook   |
| rinpola       | 1346.00     |                      | NIST Webbook   |
| ripola        | 226.44      |                      | NIST Webbook   |
| tb            | 521.00      | K                    | NIST Webbook   |
| tb            | 521.20      | K                    | NIST Webbook   |
| tc            | 769.28      | K                    | Joback Method  |
| tf            | 290.95      | K                    | Joback Method  |
| vc            | 0.509       | m <sup>3</sup> /kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 286.80 | J/mol×K | 531.57          | Joback Method |
| cpg           | 301.89 | J/mol×K | 571.19          | Joback Method |
| cpg           | 315.84 | J/mol×K | 610.81          | Joback Method |
| cpg           | 328.71 | J/mol×K | 650.43          | Joback Method |
| cpg           | 340.58 | J/mol×K | 690.05          | Joback Method |
| cpg           | 351.50 | J/mol×K | 729.66          | Joback Method |
| cpg           | 361.52 | J/mol×K | 769.28          | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C321608&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C321608&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>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>ie:</b>      | Ionization energy                               |
| <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>rinpola:</b> | Non-polar retention indices                     |
| <b>ripola:</b>  | 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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