

# Benzoic acid, 4-biphenyl ester

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C19H14O2/c20-19(17-9-5-2-6-10-17)21-18-13-11-16(12-14-18)15-7-3-1-4-8-15 |
| InchiKey:            | CINHWMYRCOGYIX-UHFFFAOYSA-N                                                       |
| Formula:             | C19H14O2                                                                          |
| SMILES:              | O=C(Oc1ccc(-c2ccccc2)cc1)c1ccccc1                                                 |
| Mol. weight [g/mol]: | 274.31                                                                            |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 202.78  | kJ/mol  | Joback Method  |
| hf            | 17.83   | kJ/mol  | Joback Method  |
| hfus          | 29.49   | kJ/mol  | Joback Method  |
| hvap          | 74.53   | kJ/mol  | Joback Method  |
| log10ws       | -6.16   |         | Crippen Method |
| logp          | 4.573   |         | Crippen Method |
| mcvol         | 214.730 | ml/mol  | McGowan Method |
| pc            | 2455.60 | kPa     | Joback Method  |
| rinpol        | 2551.00 |         | NIST Webbook   |
| rinpol        | 2551.00 |         | NIST Webbook   |
| tb            | 795.43  | K       | Joback Method  |
| tc            | 1058.56 | K       | Joback Method  |
| tf            | 467.83  | K       | Joback Method  |
| vc            | 0.799   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 590.03    | J/mol×K | 795.43          | Joback Method |
| cpg           | 605.18    | J/mol×K | 839.29          | Joback Method |
| cpg           | 618.81    | J/mol×K | 883.14          | Joback Method |
| cpg           | 631.02    | J/mol×K | 927.00          | Joback Method |
| cpg           | 641.90    | J/mol×K | 970.85          | Joback Method |
| cpg           | 651.57    | J/mol×K | 1014.71         | Joback Method |
| cpg           | 660.13    | J/mol×K | 1058.56         | Joback Method |
| dvisc         | 0.0008055 | Pa×s    | 467.83          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0004591 | Pa×s | 522.43 | Joback Method |
| dvisc | 0.0002910 | Pa×s | 577.03 | Joback Method |
| dvisc | 0.0001996 | Pa×s | 631.63 | Joback Method |
| dvisc | 0.0001454 | Pa×s | 686.23 | Joback Method |
| dvisc | 0.0001109 | Pa×s | 740.83 | Joback Method |
| dvisc | 0.0000879 | Pa×s | 795.43 | 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=U360688&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U360688&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>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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