# 4,4'-Biphthalic anhydride

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|---|---|
| **Other names:** | [5,5'-Biisobenzofuran]-1,1',3,3'-tetrone |
| | 3,3',4,4'-Biphenyltetracarboxylic acid dianhydride |
| | 4,4'-biphthalic dianhydride |
| **Inchi:** | InChI=1S/C16H6O6/c17-13-9-3-1-7(5-11(9)15(19)21-13)8-2-4-10-12(6-8)16(20)22-14(10 |
| **InchiKey:** | WKDNYTOXBCRNPV-UHFFFAOYSA-N |
| **Formula:** | C16H6O6 |
| **SMILES:** | O=C1OC(=O)c2cc(-c3ccc4c(c3)C(=O)OC4=O)ccc21 |
| **Mol. weight [g/mol]:** | 294.22 |
| **CAS:** | 2420-87-3 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -255.54 | kJ/mol | Joback Method |
| hf | -574.91 | kJ/mol | Joback Method |
| hfus | 31.85 | kJ/mol | Joback Method |
| hvap | 84.86 | kJ/mol | Joback Method |
| ie | 9.80 | eV | NIST Webbook |
| log10ws | -4.99 | | Crippen Method |
| logp | 1.975 | | Crippen Method |
| mcvol | 185.080 | ml/mol | McGowan Method |
| pc | 3443.98 | kPa | Joback Method |
| tb | 986.76 | K | Joback Method |
| tc | 1280.04 | K | Joback Method |
| tf | 743.38 | K | Joback Method |
| vc | 0.702 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 574.89 | J/mol×K | 986.76 | Joback Method |
| cpg | 582.99 | J/mol×K | 1035.64 | Joback Method |
| cpg | 588.95 | J/mol×K | 1084.52 | Joback Method |
| cpg | 592.71 | J/mol×K | 1133.40 | Joback Method |
| cpg | 594.21 | J/mol×K | 1182.28 | Joback Method |

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|---|---|---|---|---|
| cpg | 593.38 | J/mol×K | 1231.16 | Joback Method |
| cpg | 590.18 | J/mol×K | 1280.04 | Joback Method |

# Sources

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|---|---|
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2420873&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hvap:** | Enthalpy of vaporization at standard conditions |
| **ie:** | Ionization energy |
| **log10ws:** | Log10 of Water solubility in mol/l |
| **logp:** | Octanol/Water partition coefficient |
| **mcvol:** | McGowan's characteristic volume |
| **pc:** | Critical Pressure |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |