# Biphenylene

| | |
|---|---|
| **Other names:** | 1,1'-Biphenylene |
| | cyclobutadibenzene |
| | dibenzocyclobutadiene |
| | diphenylene |
| **Inchi:** | InChI=1S/C12H8/c1-2-6-10-9(5-1)11-7-3-4-8-12(10)11/h1-8H |
| **InchiKey:** | IFVTZJHWGZSXFD-UHFFFAOYSA-N |
| **Formula:** | C12H8 |
| **SMILES:** | c1ccc2c(c1)-c1ccccc1-2 |
| **Mol. weight [g/mol]:** | 152.19 |
| **CAS:** | 259-79-0 |

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| affp | 848.20 | kJ/mol | NIST Webbook |
| affp | 845.20 | kJ/mol | NIST Webbook |
| basg | 819.20 | kJ/mol | NIST Webbook |
| basg | 819.20 | kJ/mol | NIST Webbook |
| chs | -6198.85 ± 0.92 | kJ/mol | NIST Webbook |
| chs | -6219.00 ± 3.00 | kJ/mol | NIST Webbook |
| chs | -6198.00 ± 10.00 | kJ/mol | NIST Webbook |
| ea | 0.89 ± 0.10 | eV | NIST Webbook |
| gf | 360.48 | kJ/mol | Joback Method |
| hf | 440.00 | kJ/mol | NIST Webbook |
| hf | 417.20 ± 1.90 | kJ/mol | NIST Webbook |
| hf | 420.40 ± 1.90 | kJ/mol | NIST Webbook |
| hfs | 333.40 ± 1.10 | kJ/mol | NIST Webbook |
| hfs | 353.00 | kJ/mol | NIST Webbook |
| hfs | 333.40 ± 1.80 | kJ/mol | NIST Webbook |
| hfus | 22.60 | kJ/mol | Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons |
| hsub | 83.80 ± 0.30 | kJ/mol | NIST Webbook |
| hsub | 87.00 | kJ/mol | NIST Webbook |
| hsub | 87.00 ± 0.80 | kJ/mol | NIST Webbook |
| hsub | 83.80 ± 0.60 | kJ/mol | NIST Webbook |

| | | | |
|---|---|---|---|
| hsub | 87.30 ± 0.30 | kJ/mol | NIST Webbook |
| hsub | 129.00 | kJ/mol | NIST Webbook |
| hvap | 47.89 | kJ/mol | Joback Method |
| ie | 7.61 ± 0.04 | eV | NIST Webbook |
| ie | 7.53 ± 0.05 | eV | NIST Webbook |
| ie | 7.61 | eV | NIST Webbook |
| ie | 7.60 ± 0.02 | eV | NIST Webbook |
| ie | 7.56 ± 0.05 | eV | NIST Webbook |
| ie | 7.58 ± 0.03 | eV | NIST Webbook |
| ie | 7.56 ± 0.05 | eV | NIST Webbook |
| log10ws | -4.92 | | Crippen Method |
| logp | 3.334 | | Crippen Method |
| mcvol | 121.560 | ml/mol | McGowan Method |
| pc | 3673.09 | kPa | Joback Method |
| rinpol | 249.20 | | NIST Webbook |
| rinpol | 244.96 | | NIST Webbook |
| rinpol | 240.00 | | NIST Webbook |
| rinpol | 249.10 | | NIST Webbook |
| rinpol | 248.90 | | NIST Webbook |
| rinpol | 240.00 | | NIST Webbook |
| rinpol | 248.90 | | NIST Webbook |
| tb | 535.88 | K | Joback Method |
| tc | 779.55 | K | Joback Method |
| tf | 384.40 ± 0.30 | K | NIST Webbook |
| vc | 0.473 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 315.39 | J/mol×K | 738.94 | Joback Method |
| cpg | 323.61 | J/mol×K | 779.55 | Joback Method |
| cpg | 261.76 | J/mol×K | 535.88 | Joback Method |
| cpg | 274.62 | J/mol×K | 576.49 | Joback Method |
| cpg | 286.28 | J/mol×K | 617.10 | Joback Method |
| cpg | 296.86 | J/mol×K | 657.72 | Joback Method |
| cpg | 306.52 | J/mol×K | 698.33 | Joback Method |
| dvisc | 0.0007329 | Pa×s | 535.88 | Joback Method |
| dvisc | 0.0007794 | Pa×s | 502.50 | Joback Method |
| dvisc | 0.0012738 | Pa×s | 335.62 | Joback Method |
| dvisc | 0.0011143 | Pa×s | 369.00 | Joback Method |
| dvisc | 0.0009967 | Pa×s | 402.37 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0009068 | Pa×s | 435.75 | Joback Method |
| dvisc | 0.0008362 | Pa×s | 469.13 | Joback Method |
| hsubt | 68.60 ± 0.80 | kJ/mol | 295.00 | NIST Webbook |
| hsubt | 82.70 | kJ/mol | 383.00 | NIST Webbook |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C259790&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Hypothetical Thermodynamic Properties. Subcooled Vaporization Enthalpies and Vapor Pressures of Polyaromatic Hydrocarbons:** | https://www.doi.org/10.1021/je800300x |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# Legend

| | |
|---|---|
| **affp:** | Proton affinity |
| **basg:** | Gas basicity |
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **ea:** | Electron affinity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase enthalpy of formation at standard conditions |
| **hfus:** | Enthalpy of fusion at standard conditions |
| **hsub:** | Enthalpy of sublimation at standard conditions |
| **hsubt:** | Enthalpy of sublimation at a given temperature |
| **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 |
| **rinpol:** | Non-polar retention indices |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |

**vc:** Critical Volume