# 4-Bromo-2-fluorobiphenyl

**Other names:** 1,1'-Biphenyl, 4-bromo-2-fluoro-
4-bromo-2-fluoro-1,1'-biphenyl
**Inchi:** InChI=1S/C12H8BrF/c13-10-6-7-11(12(14)8-10)9-4-2-1-3-5-9/h1-8H
**InchiKey:** HTRNHWBOBYFTQF-UHFFFAOYSA-N
**Formula:** C12H8BrF
**SMILES:** Fc1cc(Br)ccc1-c1ccccc1
**Mol. weight [g/mol]:** 251.09
**CAS:** 41604-19-7

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 75.23 | kJ/mol | Joback Method |
| hf | -10.67 | kJ/mol | Joback Method |
| hfus | 22.51 | kJ/mol | Joback Method |
| hvap | 53.80 | kJ/mol | Joback Method |
| log10ws | -5.57 | | Crippen Method |
| logp | 4.255 | | Crippen Method |
| mcvol | 151.690 | ml/mol | McGowan Method |
| pc | 3403.91 | kPa | Joback Method |
| tb | 602.71 | K | Joback Method |
| tc | 855.66 | K | Joback Method |
| tf | 363.27 | K | Joback Method |
| vc | 0.572 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 323.16 | J/mol×K | 602.71 | Joback Method |
| cpg | 336.38 | J/mol×K | 644.87 | Joback Method |
| cpg | 348.49 | J/mol×K | 687.03 | Joback Method |
| cpg | 359.58 | J/mol×K | 729.19 | Joback Method |
| cpg | 369.71 | J/mol×K | 771.34 | Joback Method |
| cpg | 378.97 | J/mol×K | 813.50 | Joback Method |
| cpg | 387.43 | J/mol×K | 855.66 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C41604197&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |
| **Joback Method:** | https://en.wikipedia.org/wiki/Joback_method |

# 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 |
| **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 |