# 1,1'-Biphenyl, 2,3,3',4,4',5,5'-heptachloro-

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|---|---|
| **Other names:** | 2,3,3',4,4',5,5'-Heptachloro-1,1'-biphenyl |
| | 2,3,3',4,4',5,5'-Heptachlorobiphenyl |
| | PCB 189 |
| **Inchi:** | InChI=1S/C12H3Cl7/c13-6-1-4(2-7(14)10(6)17)5-3-8(15)11(18)12(19)9(5)16/h1-3H |
| **InchiKey:** | XUAWBXBYHDRROL-UHFFFAOYSA-N |
| **Formula:** | C12H3Cl7 |
| **SMILES:** | Clc1cc(-c2cc(Cl)c(Cl)c(Cl)c2Cl)cc(Cl)c1Cl |
| **Mol. weight [g/mol]:** | 395.32 |
| **CAS:** | 39635-31-9 |

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 124.06 | kJ/mol | Joback Method |
| hf | -8.42 | kJ/mol | Joback Method |
| hfus | 41.57 | kJ/mol | Joback Method |
| hvap | 82.19 | kJ/mol | Joback Method |
| log10ws | -8.87 | | Crippen Method |
| logp | 7.927 | | Crippen Method |
| mcvol | 218.100 | ml/mol | McGowan Method |
| pc | 2329.27 | kPa | Joback Method |
| tb | 824.19 | K | Joback Method |
| tc | 1096.84 | K | Joback Method |
| tf | 574.92 | K | Joback Method |
| vc | 0.835 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 415.14 | J/mol×K | 824.19 | Joback Method |
| cpg | 422.07 | J/mol×K | 869.63 | Joback Method |
| cpg | 428.26 | J/mol×K | 915.07 | Joback Method |
| cpg | 433.75 | J/mol×K | 960.51 | Joback Method |
| cpg | 438.58 | J/mol×K | 1005.96 | Joback Method |
| cpg | 442.79 | J/mol×K | 1051.40 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 446.42 | J/mol×K | 1096.84 | Joback Method |
| dvisc | 0.0004373 | Pa×s | 574.92 | Joback Method |
| dvisc | 0.0003321 | Pa×s | 616.47 | Joback Method |
| dvisc | 0.0002611 | Pa×s | 658.01 | Joback Method |
| dvisc | 0.0002113 | Pa×s | 699.56 | Joback Method |
| dvisc | 0.0001750 | Pa×s | 741.10 | Joback Method |
| dvisc | 0.0001479 | Pa×s | 782.64 | Joback Method |
| dvisc | 0.0001272 | Pa×s | 824.19 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C39635319&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

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |

Latest version available from:
https://www.chemeo.com/cid/93-844-2/1-1-Biphenyl-2-3-3-4-4-5-5-heptachloro.pdf
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