

1,1'-Biphenyl, 2,2',3,3'-tetrachloro-

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| Other names: | 1,2-dichloro-3-(2,3-dichlorophenyl)benzene 2,2',3,3'-PCB 2,2',3,3'-Tetrachlorobiphenyl PCB 40 |
| Inchi: | InChI=1S/C12H6Cl4/c13-9-5-1-3-7(11(9)15)8-4-2-6-10(14)12(8)16/h1-6H |
| InchiKey: | VTLYHLREPCPKX-UHFFFAOYSA-N |
| Formula: | C12H6Cl4 |
| SMILES: | Clc1cccc(-c2cccc(Cl)c2Cl)c1Cl |
| Mol. weight [g/mol]: | 291.99 |
| CAS: | 38444-93-8 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|--------------------------------------|
| gf | 188.74 | kJ/mol | Joback Method |
| hf | 73.21 | kJ/mol | Joback Method |
| hfus | 30.15 | kJ/mol | Joback Method |
| hvap | 67.05 | kJ/mol | Joback Method |
| log10ws | -7.28 | | Aqueous Solubility Prediction Method |
| log10ws | -7.28 | | Estimated Solubility Method |
| logp | 5.967 | | Crippen Method |
| mcvol | 181.380 | ml/mol | McGowan Method |
| pc | 2724.01 | kPa | Joback Method |
| rinpol | 1957.00 | | NIST Webbook |
| rinpol | 1993.00 | | NIST Webbook |
| rinpol | 1992.70 | | NIST Webbook |
| rinpol | 2000.00 | | NIST Webbook |
| rinpol | 2000.00 | | NIST Webbook |
| rinpol | 1981.40 | | NIST Webbook |
| rinpol | 1965.00 | | NIST Webbook |
| rinpol | 1965.00 | | NIST Webbook |
| rinpol | 1965.00 | | NIST Webbook |
| rinpol | 2000.00 | | NIST Webbook |
| rinpol | 2008.00 | | NIST Webbook |
| rinpol | 1993.00 | | NIST Webbook |
| rinpol | 1970.20 | | NIST Webbook |
| rinpol | 1948.00 | | NIST Webbook |

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|------|---------|----------------------|---------------|
| rinp | 1948.00 | | NIST Webbook |
| rinp | 2008.00 | | NIST Webbook |
| tb | 696.96 | K | Joback Method |
| tc | 963.35 | K | Joback Method |
| tf | 447.60 | K | Joback Method |
| vc | 0.688 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 417.60 | J/mol×K | 963.35 | Joback Method |
| cpg | 411.33 | J/mol×K | 918.95 | Joback Method |
| cpg | 404.36 | J/mol×K | 874.55 | Joback Method |
| cpg | 396.63 | J/mol×K | 830.15 | Joback Method |
| cpg | 388.08 | J/mol×K | 785.76 | Joback Method |
| cpg | 378.65 | J/mol×K | 741.36 | Joback Method |
| cpg | 368.27 | J/mol×K | 696.96 | Joback Method |
| dvisc | 0.0008409 | Paxs | 447.60 | Joback Method |
| dvisc | 0.0001717 | Paxs | 696.96 | Joback Method |
| dvisc | 0.0002057 | Paxs | 655.40 | Joback Method |
| dvisc | 0.0002526 | Paxs | 613.84 | Joback Method |
| dvisc | 0.0003196 | Paxs | 572.28 | Joback Method |
| dvisc | 0.0004195 | Paxs | 530.72 | Joback Method |
| dvisc | 0.0005766 | Paxs | 489.16 | Joback Method |
| hvapt | 81.80 | kJ/mol | 370.50 | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C38444938&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

Estimated Solubility Method: http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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 |
| h vap: | Enthalpy of vaporization at standard conditions |
| hvapt: | Enthalpy of vaporization at a given temperature |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| m cvol: | 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 |

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