

1,1'-Biphenyl, 2,3,5,6-tetrachloro-

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| Other names: | 2,3,5,6-tetrachloro-1,1'-biphenyl 2,3,5,6-tetrachlorobiphenyl PCB 65 biphenyl, 2,3,5,6-tetrachloro- |
| Inchi: | InChI=1S/C12H6Cl4/c13-8-6-9(14)12(16)10(11(8)15)7-4-2-1-3-5-7/h1-6H |
| InchiKey: | BLAYIQLVUNIICD-UHFFFAOYSA-N |
| Formula: | C12H6Cl4 |
| SMILES: | Clc1cc(Cl)c(Cl)c(-c2ccccc2)c1Cl |
| Mol. weight [g/mol]: | 291.99 |
| CAS: | 33284-54-7 |

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 | -6.81 | | Crippen Method |
| logp | 5.967 | | Crippen Method |
| mcvol | 181.380 | ml/mol | McGowan Method |
| pc | 2724.01 | kPa | Joback Method |
| tb | 696.96 | K | Joback Method |
| tc | 963.35 | K | Joback Method |
| tf | 447.60 | K | Joback Method |
| vc | 0.688 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 368.27 | J/molxK | 696.96 | Joback Method |
| cpg | 411.33 | J/molxK | 918.95 | Joback Method |
| cpg | 404.36 | J/molxK | 874.55 | Joback Method |
| cpg | 396.63 | J/molxK | 830.15 | Joback Method |
| cpg | 388.08 | J/molxK | 785.76 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 378.65 | J/molxK | 741.36 | Joback Method |
| cpg | 417.60 | J/molxK | 963.35 | 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 |
| dvisc | 0.0008409 | Paxs | 447.60 | Joback Method |

Sources

| | |
|--|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C33284547&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Henry's Law Constants for Eleven Polychlorinated Biphenyls at 20 C: | https://www.doi.org/10.1021/je0500835 |
| 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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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