

# 2,2',3,4,4'-Pentachloro-1,1'-biphenyl

<b>Other names:</b>	1,1'-Biphenyl, 2,2',3,4,4'-pentachloro 1,2,3-trichloro-4-(2,4-dichlorophenyl)benzene 2,3',4,4'-PCB PCB 85
<b>Inchi:</b>	InChI=1S/C12H5Cl5/c13-6-1-2-7(10(15)5-6)8-3-4-9(14)12(17)11(8)16/h1-5H
<b>InchiKey:</b>	LACXVZHAJMVESG-UHFFFAOYSA-N
<b>Formula:</b>	C12H5Cl5
<b>SMILES:</b>	<chem>Clc1ccc(-c2ccc(Cl)c(Cl)c2Cl)c(Cl)c1</chem>
<b>Mol. weight [g/mol]:</b>	326.43
<b>CAS:</b>	65510-45-4

## Physical Properties

Property code	Value	Unit	Source
gf	167.18	kJ/mol	Joback Method
hf	46.00	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	72.09	kJ/mol	Joback Method
log10ws	-7.80		Estimated Solubility Method
log10ws	-7.80		Aqueous Solubility Prediction Method
logp	6.621		Crippen Method
mvol	193.620	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	2179.00		NIST Webbook
rinpol	2179.00		NIST Webbook
rinpol	2188.00		NIST Webbook
rinpol	2188.00		NIST Webbook
tb	739.37	K	Joback Method
tc	1008.22	K	Joback Method
tf	490.04	K	Joback Method
vc	0.737	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.50	J/molxK	739.37	Joback Method
cpg	394.64	J/molxK	784.18	Joback Method
cpg	402.91	J/molxK	828.99	Joback Method
cpg	410.38	J/molxK	873.79	Joback Method
cpg	417.08	J/molxK	918.60	Joback Method
cpg	423.09	J/molxK	963.41	Joback Method
cpg	428.46	J/molxK	1008.22	Joback Method
dvisc	0.0006694	Paxs	490.04	Joback Method
dvisc	0.0004783	Paxs	531.60	Joback Method
dvisc	0.0003588	Paxs	573.15	Joback Method
dvisc	0.0002798	Paxs	614.71	Joback Method
dvisc	0.0002252	Paxs	656.26	Joback Method
dvisc	0.0001860	Paxs	697.82	Joback Method
dvisc	0.0001570	Paxs	739.37	Joback Method

## Sources

**McGowan Method:**

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

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C65510454&Units=SI>

**Crippen Method:**

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

**Joback Method:**

[https://en.wikipedia.org/wiki/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](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mccvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices

**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature  
**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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