

# 1,1'-Biphenyl, 2,4,4',6-tetrachloro-

<b>Other names:</b>	2,4,4',6-Tetrachloro-1,1'-biphenyl 2,4,4',6-tetrachlorobiphenyl 2,4,4'6-Tetrachlorobiphenyl PCB 75
<b>Inchi:</b>	InChI=1S/C12H6Cl4/c13-8-3-1-7(2-4-8)12-10(15)5-9(14)6-11(12)16/h1-6H
<b>InchiKey:</b>	RZfZBHKDGHISsh-UHFFFAOYSA-N
<b>Formula:</b>	C12H6Cl4
<b>SMILES:</b>	Clc1ccc(-c2c(Cl)cc(Cl)cc2Cl)cc1
<b>Mol. weight [g/mol]:</b>	291.99
<b>CAS:</b>	32598-12-2

## Physical Properties

Property code	Value	Unit	Source
gf	188.74	kJ/mol	Joback Method
hf	73.21	kJ/mol	Joback Method
h <sub>fus</sub>	30.15	kJ/mol	Joback Method
h <sub>vap</sub>	67.05	kJ/mol	Joback Method
log <sub>10</sub> ws	-6.94		Aqueous Solubility Prediction Method
logp	5.967		Crippen Method
m <sub>cvol</sub>	181.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
r <sub>inpol</sub>	1898.00		NIST Webbook
r <sub>inpol</sub>	1898.00		NIST Webbook
tb	696.96	K	Joback Method
tc	963.35	K	Joback Method
tf	447.60	K	Joback Method
vc	0.688	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
c <sub>pg</sub>	368.27	J/mol×K	696.96	Joback Method
c <sub>pg</sub>	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	417.60	J/mol×K	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

**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>

**McGowan Method:**

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

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C32598122&Units=SI>

**Crippen Method:**

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

## 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>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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