

# 1,1'-Biphenyl, 3,3',4,4'-tetrachloro-

<b>Other names:</b>	3,3',4,4'-Tetrachloro-1,1'-biphenyl 3,3',4,4'-Tetrachlorobiphenyl 3,4,3',4'-Tetrachlorobiphenyl 4-CB Biphenyl, 3,3',4,4'-tetrachloro- PCB 77 TCB
<b>Inchi:</b>	InChI=1S/C12H6Cl4/c13-9-3-1-7(5-11(9)15)8-2-4-10(14)12(16)6-8/h1-6H
<b>InchiKey:</b>	UQMGIJOKDKOLIDP-UHFFFAOYSA-N
<b>Formula:</b>	C12H6Cl4
<b>SMILES:</b>	Clc1ccc(-c2ccc(Cl)c(Cl)c2)cc1Cl
<b>Mol. weight [g/mol]:</b>	291.99
<b>CAS:</b>	32598-13-3

## 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	-8.53		Aqueous Solubility Prediction Method
logp	5.967		Crippen Method
mcvol	181.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	2237.00		NIST Webbook
rinpol	2236.00		NIST Webbook
rinpol	2234.00		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	2228.00		NIST Webbook
rinpol	2231.20		NIST Webbook
rinpol	2146.60		NIST Webbook
rinpol	2147.10		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
cpg	411.33	J/molxK	918.95	Joback Method
cpg	417.60	J/molxK	963.35	Joback Method
cpg	368.27	J/molxK	696.96	Joback Method
cpg	378.65	J/molxK	741.36	Joback Method
cpg	388.08	J/molxK	785.76	Joback Method
cpg	396.63	J/molxK	830.15	Joback Method
cpg	404.36	J/molxK	874.55	Joback Method
dvisc	0.0001717	Paxs	696.96	Joback Method
dvisc	0.0002057	Paxs	655.40	Joback Method
dvisc	0.0008409	Paxs	447.60	Joback Method
dvisc	0.0005766	Paxs	489.16	Joback Method
dvisc	0.0004195	Paxs	530.72	Joback Method
dvisc	0.0003196	Paxs	572.28	Joback Method
dvisc	0.0002526	Paxs	613.84	Joback Method
hsubt	121.60 ± 1.30	kJ/mol	393.00	NIST Webbook
hvapt	87.20	kJ/mol	368.00	NIST Webbook

## Sources

**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=C32598133&Units=SI>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307i>

**Joback Method:** [https://en.wikipedia.org/wiki/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

<b>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>h vap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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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