

# 1,1'-Biphenyl, 2,2',3,3',5,5'-Hexachloro-

<b>Other names:</b>	2,2',3,3',5,5'-Hexachlorobiphenyl 2,2',4,4',5,5'-Hexachlorobiphenyl PCB 133
<b>Inchi:</b>	InChI=1S/C12H4Cl6/c13-5-1-7(11(17)9(15)3-5)8-2-6(14)4-10(16)12(8)18/h1-4H
<b>InchiKey:</b>	AJKLKINFZLWHQE-UHFFFAOYSA-N
<b>Formula:</b>	C12H4Cl6
<b>SMILES:</b>	Clc1cc(Cl)c(Cl)c(-c2cc(Cl)cc(Cl)c2Cl)c1
<b>Mol. weight [g/mol]:</b>	360.88
<b>CAS:</b>	35694-04-3

## Physical Properties

Property code	Value	Unit	Source
gf	145.62	kJ/mol	Joback Method
hf	18.79	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	77.14	kJ/mol	Joback Method
log10ws	-7.25		Aqueous Solubility Prediction Method
logp	7.274		Crippen Method
mcvol	205.860	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2206.00		NIST Webbook
rinpol	2281.00		NIST Webbook
rinpol	2206.00		NIST Webbook
rinpol	2283.00		NIST Webbook
tb	781.78	K	Joback Method
tc	1052.68	K	Joback Method
tf	532.48	K	Joback Method
vc	0.785	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.07	J/molxK	781.78	Joback Method

cpg	409.07	J/mol×K	826.93	Joback Method
cpg	416.26	J/mol×K	872.08	Joback Method
cpg	422.71	J/mol×K	917.23	Joback Method
cpg	428.46	J/mol×K	962.38	Joback Method
cpg	433.56	J/mol×K	1007.53	Joback Method
cpg	438.05	J/mol×K	1052.68	Joback Method
dvisc	0.0005388	Paxs	532.48	Joback Method
dvisc	0.0003981	Paxs	574.03	Joback Method
dvisc	0.0003063	Paxs	615.58	Joback Method
dvisc	0.0002437	Paxs	657.13	Joback Method
dvisc	0.0001992	Paxs	698.68	Joback Method
dvisc	0.0001666	Paxs	740.23	Joback Method
dvisc	0.0001419	Paxs	781.78	Joback Method
hfust	29.20	kJ/mol	424.90	NIST Webbook

## Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C35694043&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C35694043&amp;Units=SI</a>

## 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>hfust:</b>	Enthalpy of fusion at a given temperature
<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

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

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