1,1'-Biphenyl, 2,2',4,5'-tetrachloro-

Other names:	1,1'-Biphenyl, 2,2',4',5-tetrachloro
	2,2',4,5'-PCB
	2,2',4,5'-Tetrachlorobiphenyl
	2,4,2',5'-Tetrachlorobiphenyl
	2,4-dichloro-1-(2,5-dichlorophenyl)benzene
	PCB 49
Inchi:	InChI=1S/C12H6Cl4/c13-7-2-4-11(15)10(5-7)9-3-1-8(14)6-12(9)16/h1-6H
InchiKey:	ZWPVHELAQPIZHO-UHFFFAOYSA-N
Formula:	C12H6Cl4
SMILES:	Clc1ccc(-c2cc(Cl)ccc2Cl)c(Cl)c1
Mol. weight [g/mol]:	291.99
CAS:	41464-40-8

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	87.40 ± 0.80	kJ/mol	NIST Webbook
log10ws	-6.57		Estimated Solubility Method
log10ws	-6.57		Aqueous Solubility Prediction Method
logp	5.967		Crippen Method
mcvol	181.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1909.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1937.00		NIST Webbook
rinpol	1971.00		NIST Webbook
rinpol	1895.00		NIST Webbook
rinpol	1972.00		NIST Webbook
rinpol	1890.00		NIST Webbook
rinpol	1931.30		NIST Webbook
rinpol	1937.00		NIST Webbook

rinpol	1909.00		NIST Webbook
rinpol	1931.30		NIST Webbook
rinpol	1931.70		NIST Webbook
rinpol	1921.60		NIST Webbook
rinpol	1911.80		NIST Webbook
rinpol	1891.00		NIST Webbook
rinpol	1890.00		NIST Webbook
tb	696.96	K	Joback Method
tc	963.35	K	Joback Method
tf	339.10 ± 0.20	K	NIST Webbook
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.27	J/mol×K	696.96	Joback Method
cpg	378.65	J/mol×K	741.36	Joback Method
cpg	388.08	J/mol×K	785.76	Joback Method
cpg	396.63	J/mol×K	830.15	Joback Method
cpg	404.36	J/mol×K	874.55	Joback Method
cpg	411.33	J/mol×K	918.95	Joback Method
cpg	417.60	J/mol×K	963.35	Joback Method
dvisc	0.0008409	Pa×s	447.60	Joback Method
dvisc	0.0005766	Pa×s	489.16	Joback Method
dvisc	0.0004195	Pa×s	530.72	Joback Method
dvisc	0.0003196	Pa×s	572.28	Joback Method
dvisc	0.0002526	Pa×s	613.84	Joback Method
dvisc	0.0002057	Pa×s	655.40	Joback Method
dvisc	0.0001717	Pa×s	696.96	Joback Method
hfust	23.40	kJ/mol	339.10	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41464408&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

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
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume