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

Other names:	1,4-dichloro-2-(2,5-dichlorophenyl)benzene
	2,2',5,5'-TCB
	2,2',5,5'-Tetrachloro-1,1'-biphenyl
	2,2',5,5'-Tetrachlorobiphenyl
	2,5,2',5'-Tetrachlorobiphenyl
	PCB-52
Inchi:	InChI=1S/C12H6Cl4/c13-7-1-3-11(15)9(5-7)10-6-8(14)2-4-12(10)16/h1-6H
InchiKey:	HCWZEPKLWVAEOV-UHFFFAOYSA-N
Formula:	C12H6Cl4
SMILES:	Clc1ccc(Cl)c(-c2cc(Cl)ccc2Cl)c1
Mol. weight [g/mol]:	291.99
CAS:	35693-99-3

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	-7.00		Aqueous Solubility Prediction Method
logp	5.967		Crippen Method
mcvol	181.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1884.00		NIST Webbook
rinpol	1913.30		NIST Webbook
rinpol	1923.10		NIST Webbook
rinpol	1922.70		NIST Webbook
rinpol	1909.80		NIST Webbook
rinpol	1900.40		NIST Webbook
rinpol	1900.00		NIST Webbook
rinpol	1886.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1903.70		NIST Webbook
rinpol	1935.00		NIST Webbook

rinpol	1887.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1964.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1956.00		NIST Webbook
rinpol	1955.00		NIST Webbook
tb	696.96	K	Joback Method
tc	963.35	K	Joback Method
tf	447.60	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	411.33	J/mol×K	918.95	Joback Method
cpg	388.08	J/mol×K	785.76	Joback Method
cpg	378.65	J/mol×K	741.36	Joback Method
cpg	368.27	J/mol×K	696.96	Joback Method
cpg	396.63	J/mol×K	830.15	Joback Method
cpg	417.60	J/mol×K	963.35	Joback Method
cpg	404.36	J/mol×K	874.55	Joback Method
dvisc	0.0008409	Pa×s	447.60	Joback Method
dvisc	0.0001717	Pa×s	696.96	Joback Method
dvisc	0.0002057	Pa×s	655.40	Joback Method
dvisc	0.0002526	Pa×s	613.84	Joback Method
dvisc	0.0003196	Pa×s	572.28	Joback Method
dvisc	0.0004195	Pa×s	530.72	Joback Method
dvisc	0.0005766	Pa×s	489.16	Joback Method
hsubt	94.60	kJ/mol	307.50	NIST Webbook
hsubt	102.00 ± 0.50	kJ/mol	338.00	NIST Webbook
hvapt	79.00	kJ/mol	398.00	NIST Webbook
hvapt	80.80	kJ/mol	370.50	NIST Webbook

Sources

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

Henry's Law Constants for Eleven Polychlorinated Biphenyls at 20 C: https://www.doi.org/10.1021/je0500835

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=C35693993&Units=SI

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
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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