1,1'-Biphenyl, 2,2',3,3',4,4',5,5'-octachloro-

Other names:	1,2,3,4-tetrachloro-5-(2,3,4,5-tetrachlorophenyl)benzene
	2,2',3,3',4,4',5,5'-Octachloro-1,1'-biphenyl
	2,2',3,3',4,4',5,5'-Octachlorobiphenyl
	2,2',3,3',4,4',5,5'-PCB
	2,3,4,5,2',3',4',5'-Octachlorobiphenyl
	PCB 194
Inchi:	InChI=1S/C12H2Cl8/c13-5-1-3(7(15)11(19)9(5)17)4-2-6(14)10(18)12(20)8(4)16/h1-2H
InchiKey:	DTMRKGRREZAYAP-UHFFFAOYSA-N
Formula:	C12H2Cl8
SMILES:	Clc1cc(-c2cc(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	429.77
CAS:	35694-08-7

Physical Properties

Property code	Value	Unit	Source
gf	102.50	kJ/mol	Joback Method
hf	-35.63	kJ/mol	Joback Method
hfus	45.38	kJ/mol	Joback Method
hvap	87.23	kJ/mol	Joback Method
log10ws	-9.16		Aqueous Solubility Prediction Method
log10ws	-9.16		Estimated Solubility Method
logp	8.581		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
tb	866.60	K	Joback Method
tc	1140.81	K	Joback Method
tf	617.36	K	Joback Method
vc	0.883	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	427.83	J/mol×K	866.60	Joback Method
cpg	450.83	J/mol×K	1095.11	Joback Method
cpg	447.49	J/mol×K	1049.40	Joback Method
cpg	443.56	J/mol×K	1003.70	Joback Method
cpg	438.99	J/mol×K	958.00	Joback Method
cpg	433.76	J/mol×K	912.30	Joback Method
cpg	453.59	J/mol×K	1140.81	Joback Method
dvisc	0.0001131	Pa×s	866.60	Joback Method
dvisc	0.0001305	Pa×s	825.06	Joback Method
dvisc	0.0001530	Pa×s	783.52	Joback Method
dvisc	0.0001825	Pa×s	741.98	Joback Method
dvisc	0.0002223	Pa×s	700.44	Joback Method
dvisc	0.0002775	Pa×s	658.90	Joback Method
dvisc	0.0003571	Pa×s	617.36	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C35694087&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

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

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
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
tb: Normal Boiling Point Temperature
tc: Critical Temperature

tf: Normal melting (fusion) point

vc: Critical Volume