1,1'-Biphenyl, 2,2',3,3',4,4',6,6'-octachloro-

Other names:	Biphenyl, 2,2',3,3',4,4',6,6'-octachloro-
	2,2',3,3',4,4',6,6'-Octachlorobiphenyl
	2,2',3,3',4,4',6,6'-Octachloro-1,1'-biphenyl
	PCB 197
Inchi:	InChI=1S/C12H2Cl8/c13-3-1-5(15)9(17)11(19)7(3)8-4(14)2-6(16)10(18)12(8)20/h1-2H
InchiKey:	YPDBBDKYNWRFMF-UHFFFAOYSA-N
Formula:	C12H2Cl8
SMILES:	Clc1cc(Cl)c(-c2c(Cl)cc(Cl)c(Cl)c2Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	429.77
CAS:	33091-17-7

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	-9.55		Crippen Method
logp	8.581		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	2462.00		NIST Webbook
rinpol	2471.00		NIST Webbook
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	433.76	J/mol×K	912.30	Joback Method
cpg	438.99	J/mol×K	958.00	Joback Method

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

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C33091177&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
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