1,1'-Biphenyl, 2,2',3,3',5,5',6,6'-octachloro-

Other names:	1,2,4,5-tetrachloro-3-(2,3,5,6-tetrachlorophenyl)benzene
	2,2',3,3',5,5',6,6'-Octachloro-1,1'-biphenyl
	2,2',3,3',5,5',6,6'-Octachlorobiphenyl
	2,2',3,3',5,5',6,6'-PCB
	2,3,5,6,2',3',5',6'-Octachlorobiphenyl
	Biphenyl, 2,2',3,3',5,5',6,6'-octachloro-
	PCB 202
Inchi:	InChI=1S/C12H2Cl8/c13-3-1-4(14)10(18)7(9(3)17)8-11(19)5(15)2-6(16)12(8)20/h1-2H
InchiKey:	JPOPEORRMSDUIP-UHFFFAOYSA-N
Formula:	C12H2Cl8
SMILES:	Clc1cc(Cl)c(Cl)c(-c2c(Cl)c(Cl)cc(Cl)c2Cl)c1Cl
Mol. weight [g/mol]:	429.77
CAS:	2136-99-4

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	-9.15		Aqueous Solubility Prediction Method
log10ws	-9.15		Estimated Solubility Method
logp	8.581		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
pc	2216.62	kPa	Joback Method
rinpol	2391.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2381.00		NIST Webbook
rinpol	2403.00		NIST Webbook
rinpol	2410.00		NIST Webbook
rinpol	2381.00		NIST Webbook
tb	866.60	K	Joback Method
tc	1140.81	K	Joback Method
tf	433.80 ± 0.20	K	NIST Webbook

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	0.0001131	Pa×s	866.60	Joback Method
dvisc	0.0002775	Pa×s	658.90	Joback Method
dvisc	0.0003571	Pa×s	617.36	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	0.0002223	Pa×s	700.44	Joback Method
hfust	22.80	kJ/mol	433.80	NIST Webbook
hfust	22.80	kJ/mol	433.80	NIST Webbook
hsubt	101.70	kJ/mol	318.00	NIST Webbook
hvapt	92.90	kJ/mol	368.00	NIST Webbook
hvapt	92.90	kJ/mol	398.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2136994&Units=SI

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

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
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

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