Decachlorobiphenyl

Other names:	1,1'-Biphenyl, 2,2',3,3',4,4',5,5',6,6'-decachloro-
	1,2,3,4,5-pentachloro-6-(2,3,4,5,6-pentachlorophenyl)benzene
	2,2',3,3',4,4', 5,5',6,6'-Decachlorobiphenyl
	2,2',3,3',4,4',5,5',6,6'-Decachloro-1,1'-biphenyl
	2,2',3,3',4,4',5,5',6,6'-PCB
	Biphenyl, decachloro-
	Dcb
	Pcb 209
	Perchlorobiphenyl
	decachloro-1,1'-biphenyl
Inchi:	InChI=1S/C12Cl10/c13-3-1(4(14)8(18)11(21)7(3)17)2-5(15)9(19)12(22)10(20)6(2)16
InchiKey:	ONXPZLFXDMAPRO-UHFFFAOYSA-N
Formula:	C12Cl10
SMILES:	Clc1c(Cl)c(Cl)c(-c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	498.66
CAS:	2051-24-3

Physical Properties

Property code	Value	Unit	Source
gf	59.38	kJ/mol	Joback Method
hf	-90.05	kJ/mol	Joback Method
hfus	53.00	kJ/mol	Joback Method
hvap	97.33	kJ/mol	Joback Method
log10ws	-11.60		Estimated Solubility Method
log10ws	-11.62		Aqueous Solubility Prediction Method
logp	9.888		Crippen Method
mcvol	254.820	ml/mol	McGowan Method
pc	2014.51	kPa	Joback Method
rinpol	460.18		NIST Webbook
rinpol	460.18		NIST Webbook
ss	455.80	J/mol×K	NIST Webbook
tb	951.42	K	Joback Method
tc	1228.57	K	Joback Method
tf	580.66 ± 0.20	K	NIST Webbook
tf	577.65 ± 2.00	K	NIST Webbook

tf	578.90 ± 0.20	K	NIST Webbook
tf	578.95	K	Aqueous Solubility Prediction Method
vc	0.982	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	464.14	J/mol×K	1228.57	Joback Method
cpg	463.24	J/mol×K	1182.38	Joback Method
cpg	461.74	J/mol×K	1136.19	Joback Method
cpg	459.62	J/mol×K	1090.00	Joback Method
cpg	456.87	J/mol×K	1043.80	Joback Method
cpg	453.48	J/mol×K	997.61	Joback Method
cpg	449.43	J/mol×K	951.42	Joback Method
cps	344.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0001153	Pa×s	868.36	Joback Method
dvisc	0.0001349	Pa×s	826.83	Joback Method
dvisc	0.0000878	Pa×s	951.42	Joback Method
dvisc	0.0002411	Pa×s	702.24	Joback Method
dvisc	0.0001944	Pa×s	743.77	Joback Method
dvisc	0.0001604	Pa×s	785.30	Joback Method
dvisc	0.0001000	Pa×s	909.89	Joback Method
hfust	39.34	kJ/mol	577.70	NIST Webbook
hfust	39.34	kJ/mol	577.70	NIST Webbook
hfust	41.20	kJ/mol	580.30	NIST Webbook
hsubt	121.80	kJ/mol	343.50	NIST Webbook
hvapt	103.40	kJ/mol	398.00	NIST Webbook
hvapt	103.40	kJ/mol	368.00	NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051243&Units=SI

Legend

cpg:	Ideal gas heat capacity
cps:	Solid phase 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
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume