1,1'-Biphenyl, 4,4'-dichloro-

Other names:	1-chloro-4-(4-chlorophenyl)benzene
	4,4'-Dichloro-1,1'-biphenyl
	4,4'-Dichlorobiphenyl
	4,4'-PCB
	Biphenyl, 4,4'-dichloro-
	PCB 15
	p,p'-Dichlorobiphenyl
	p,p-DCBP
Inchi:	InChI=1S/C12H8Cl2/c13-11-5-1-9(2-6-11)10-3-7-12(14)8-4-10/h1-8H
InchiKey:	YTBRNEUEFCNVHC-UHFFFAOYSA-N
Formula:	C12H8Cl2
SMILES:	Clc1ccc(-c2ccc(Cl)cc2)cc1
Mol. weight [g/mol]:	223.10
CAS:	2050-68-2

Physical Properties

Property code	Value	Unit	Source
chs	-5813.54	kJ/mol	NIST Webbook
chs	-5927.10 ± 0.63	kJ/mol	NIST Webbook
gf	231.86	kJ/mol	Joback Method
hf	120.00	kJ/mol	NIST Webbook
hfs	16.50	kJ/mol	NIST Webbook
hfus	22.53	kJ/mol	Joback Method
hsub	104.00 ± 4.20	kJ/mol	NIST Webbook
hsub	91.20 ± 4.20	kJ/mol	NIST Webbook
hsub	103.80 ± 4.20	kJ/mol	NIST Webbook
hvap	81.40 ± 0.30	kJ/mol	NIST Webbook
log10ws	-6.56		Estimated Solubility Method
log10ws	-6.56		Aqueous Solubility Prediction Method
logp	4.660		Crippen Method
mcvol	156.900	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1776.00		NIST Webbook

rinpol	1746.00		NIST Webbook
rinpol	1781.80		NIST Webbook
rinpol	1792.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1743.00		NIST Webbook
rinpol	1788.00		NIST Webbook
rinpol	1772.30		NIST Webbook
rinpol	1762.90		NIST Webbook
rinpol	1781.80		NIST Webbook
rinpol	1735.00		NIST Webbook
tb	590.20	K	NIST Webbook
tc	871.88	K	Joback Method
tf	420.00 ± 3.00	K	NIST Webbook
tf	422.50 ± 2.00	K	NIST Webbook
tf	422.25	K	Aqueous Solubility Prediction Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	328.07	J/mol×K	612.14	Joback Method
cpg	341.24	J/mol×K	655.43	Joback Method
cpg	353.28	J/mol×K	698.72	Joback Method
cpg	364.26	J/mol×K	742.01	Joback Method
cpg	374.26	J/mol×K	785.30	Joback Method
cpg	383.35	J/mol×K	828.59	Joback Method
cpg	391.60	J/mol×K	871.88	Joback Method
dvisc	0.0005691	Pa×s	445.86	Joback Method
dvisc	0.0008516	Pa×s	404.29	Joback Method
dvisc	0.0013975	Pa×s	362.72	Joback Method
dvisc	0.0004074	Pa×s	487.43	Joback Method
dvisc	0.0003074	Pa×s	529.00	Joback Method
dvisc	0.0002417	Pa×s	570.57	Joback Method
dvisc	0.0001963	Pa×s	612.14	Joback Method
hsubt	95.30 ± 1.30	kJ/mol	283.00	NIST Webbook
hsubt	103.70	kJ/mol	331.50	NIST Webbook
hsubt	91.40	kJ/mol	306.00	NIST Webbook
hvapt	76.00	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=C2050682&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hsub:	Enthalpy of sublimation 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