1,1'-Biphenyl, 4-chloro-

Other names:	1-Chloro-4-phenylbenzene
	4-Chloro-1,1'-biphenyl
	4-Chlorobiphenyl
	4-Chlorodiphenyl
	Biphenyl, 4-chloro-
	PCB 3
	p-Chlorobiphenyl
	p-Chlorodiphenyl
Inchi:	InChI=1S/C12H9Cl/c13-12-8-6-11(7-9-12)10-4-2-1-3-5-10/h1-9H
InchiKey:	FPWNLURCHDRMHC-UHFFFAOYSA-N
Formula:	C12H9Cl
SMILES:	Clc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	188.65
CAS:	2051-62-9

Physical Properties

Property code	Value	Unit	Source
chs	-6040.06	kJ/mol	NIST Webbook
gf	253.42	kJ/mol	Joback Method
hf	154.84	kJ/mol	Joback Method
hfus	18.73	kJ/mol	Joback Method
hvap	71.60 ± 0.70	kJ/mol	NIST Webbook
ie	8.10 ± 0.02	eV	NIST Webbook
log10ws	-5.18		Aqueous Solubility Prediction Method
logp	4.007		Crippen Method
mcvol	144.660	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	1542.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1564.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1548.00		NIST Webbook
rinpol	1549.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1586.00		NIST Webbook
rinpol	1564.00		NIST Webbook

rinpol	1586.00		NIST Webbook
ss	256.90	J/mol×K	NIST Webbook
ss	256.90	J/mol×K	NIST Webbook
tb	555.00	K	NIST Webbook
tb	564.20	K	NIST Webbook
tc	825.02	K	Joback Method
tf	351.42	K	Aqueous Solubility Prediction Method
tt	348.55 ± 0.02	K	NIST Webbook
tt	348.55 ± 0.02	K	NIST Webbook
tt	347.90 ± 0.10	K	NIST Webbook
vc	0.540	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	376.10	J/mol×K	825.02	Joback Method
cpg	304.63	J/mol×K	569.73	Joback Method
cpg	366.74	J/mol×K	782.47	Joback Method
cpg	356.46	J/mol×K	739.92	Joback Method
cpg	345.19	J/mol×K	697.37	Joback Method
cpg	332.84	J/mol×K	654.83	Joback Method
cpg	319.35	J/mol×K	612.28	Joback Method
cps	243.80	J/mol×K	298.15	NIST Webbook
cps	243.76	J/mol×K	298.15	NIST Webbook
dvisc	0.0002543	Pa×s	528.15	Joback Method
dvisc	0.0010478	Pa×s	361.85	Joback Method
dvisc	0.0006592	Pa×s	403.43	Joback Method
dvisc	0.0004522	Pa×s	445.00	Joback Method
dvisc	0.0002031	Pa×s	569.73	Joback Method
dvisc	0.0018784	Pa×s	320.28	Joback Method
dvisc	0.0003309	Pa×s	486.58	Joback Method
hfust	13.32	kJ/mol	348.60	NIST Webbook
hfust	13.32	kJ/mol	348.55	NIST Webbook
hfust	13.32	kJ/mol	348.60	NIST Webbook
hfust	13.32	kJ/mol	348.55	NIST Webbook
hsubt	86.00 ± 0.90	kJ/mol	278.00	NIST Webbook
hsubt	73.70 ± 0.70	kJ/mol	326.00	NIST Webbook
hvapt	59.00	kJ/mol	467.50	NIST Webbook
hvapt	65.90	kJ/mol	493.50	NIST Webbook
hvapt	66.80	kJ/mol	368.00	NIST Webbook

hvapt	67.80	kJ/mol	378.50	NIST Webbook
sfust	38.21	J/mol×K	348.55	NIST Webbook
sfust	38.21	J/mol×K	348.55	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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2051629&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
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
ie:	Ionization energy
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
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume