1,1'-Biphenyl, 2,2'-dichloro-

Other names:	1-chloro-2-(2-chlorophenyl)benzene
	2,2'-Dichlorbiphenyl
	2,2'-Dichloro-1,1'-biphenyl
	2,2'-Dichlorobiphenyl
	2,2'-Dichlorodiphenyl
	2,2'-PCB
	Biphenyl, 2,2'-dichloro-
	O,O'-Dichlorobiphenyl
	PCB 4
Inchi:	InChI=1S/C12H8Cl2/c13-11-7-3-1-5-9(11)10-6-2-4-8-12(10)14/h1-8H
InchiKey:	JAYCNKDKIKZTAF-UHFFFAOYSA-N
Formula:	C12H8Cl2
SMILES:	Clc1ccccc1-c1ccccc1Cl
Mol. weight [g/mol]:	223.10
CAS:	13029-08-8

Physical Properties

Property code	Value	Unit	Source
chs	-5831.91	kJ/mol	NIST Webbook
chs	-5941.50 ± 1.70	kJ/mol	NIST Webbook
gf	231.86	kJ/mol	Joback Method
hf	127.90 ± 4.80	kJ/mol	NIST Webbook
hfs	31.70 ± 2.30	kJ/mol	NIST Webbook
hfus	22.53	kJ/mol	Joback Method
hsub	96.20 ± 4.20	kJ/mol	NIST Webbook
hsub	96.20 ± 4.20	kJ/mol	NIST Webbook
hvap	56.95	kJ/mol	Joback Method
log10ws	-5.27		Aqueous Solubility Prediction Method
log10ws	-5.27		Estimated Solubility Method
logp	4.660		Crippen Method
mcvol	156.900	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1620.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1553.00		NIST Webbook

rinpol	1606.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1631.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1625.80		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1553.00		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1606.00		NIST Webbook
tb	612.14	K	Joback Method
tc	871.88	K	Joback Method
tf	334.65	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	0.0008516	Pa×s	404.29	Joback Method
dvisc	0.0013975	Pa×s	362.72	Joback Method
dvisc	0.0005691	Pa×s	445.86	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	87.80 ± 1.20	kJ/mol	313.00	NIST Webbook
hsubt	96.10	kJ/mol	319.00	NIST Webbook

Sources

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=C13029088&Units=SI
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

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
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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