

1,1'-Biphenyl, 2,6-dichloro-

Other names:	1,3-dichloro-2-phenylbenzene 2,6-Dichloro-1,1'-biphenyl 2,6-Dichlorobiphenyl 2,6-PCB Biphenyl, 2,6-dichloro- PCB 10
Inchi:	InChI=1S/C12H8Cl2/c13-10-7-4-8-11(14)12(10)9-5-2-1-3-6-9/h1-8H
InchiKey:	IYZWUWBAFUBNCH-UHFFFAOYSA-N
Formula:	C12H8Cl2
SMILES:	Clc1cccc(Cl)c1-c1ccccc1
Mol. weight [g/mol]:	223.10
CAS:	33146-45-1

Physical Properties

Property code	Value	Unit	Source
gf	231.86	kJ/mol	Joback Method
hf	127.63	kJ/mol	Joback Method
hfus	22.53	kJ/mol	Joback Method
hvap	56.95	kJ/mol	Joback Method
log10ws	-5.21		Aqueous Solubility Prediction Method
log10ws	-5.21		Estimated Solubility Method
logp	4.660		Crippen Method
mcvol	156.900	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1618.60		NIST Webbook
rinpol	1590.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1610.10		NIST Webbook
rinpol	1620.00		NIST Webbook
rinpol	1627.90		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1580.00		NIST Webbook
rinpol	1560.00		NIST Webbook

rinpol	1562.00		NIST Webbook
rinpol	1591.00		NIST Webbook
rinpol	1639.00		NIST Webbook
tb	612.14	K	Joback Method
tc	871.88	K	Joback Method
tf	307.90 ± 0.20	K	NIST Webbook
vc	0.590	m ³ /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
hfust	12.60	kJ/mol	307.90	NIST Webbook
hfust	12.60	kJ/mol	307.90	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/AqueousDataset002.xlsx
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=C33146451&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
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
rmpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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