

1,1'-Biphenyl, 2,4-dichloro-

Other names:	2,4-Dichloro-1,1'-biphenyl 2,4-Dichloro-1-phenylbenzene 2,4-Dichlorobiphenyl Biphenyl, 2,4-dichloro- PCB 7
Inchi:	InChI=1S/C12H8Cl2/c13-10-6-7-11(12(14)8-10)9-4-2-1-3-5-9/h1-8H
InchiKey:	WEJZHJJPXXMU-UHFFFAOYSA-N
Formula:	C12H8Cl2
SMILES:	Clc1ccc(-c2ccccc2)c(Cl)c1
Mol. weight [g/mol]:	223.10
CAS:	33284-50-3

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	75.30 ± 1.50	kJ/mol	NIST Webbook
log10ws	-5.25		Aqueous Solubility Prediction Method
logp	4.660		Crippen Method
mcvol	156.900	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1653.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1646.00		NIST Webbook
rinpol	1643.00		NIST Webbook
rinpol	1637.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1638.00		NIST Webbook
rinpol	1628.00		NIST Webbook
rinpol	1653.00		NIST Webbook
rinpol	1630.00		NIST Webbook
rinpol	1667.00		NIST Webbook
rinpol	1671.40		NIST Webbook
tb	612.14	K	Joback Method
tc	871.88	K	Joback Method

tf	362.72	K	Joback Method
vc	0.590	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	391.60	J/mol×K	871.88	Joback Method
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
dvisc	0.0001963	Pa×s	612.14	Joback Method
dvisc	0.0013975	Pa×s	362.72	Joback Method
dvisc	0.0008516	Pa×s	404.29	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
hvapt	73.50	kJ/mol	368.00	NIST Webbook

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C33284503&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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
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

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