

1,1'-Biphenyl, 3,4-dichloro-

Other names:	1,2-dichloro-4-phenylbenzene 3,4-Dichloro-1,1'-biphenyl 3,4-Dichlorobiphenyl 3,4-PCB Biphenyl, 3,4-dichloro- PCB 12
Inchi:	InChI=1S/C12H8Cl2/c13-11-7-6-10(8-12(11)14)9-4-2-1-3-5-9/h1-8H
InchiKey:	ZGHQUYZPMWMLBM-UHFFFAOYSA-N
Formula:	C12H8Cl2
SMILES:	Clc1ccc(-c2ccccc2)cc1Cl
Mol. weight [g/mol]:	223.10
CAS:	2974-92-7

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	-6.39		Estimated Solubility Method
log10ws	-6.39		Aqueous Solubility Prediction Method
logp	4.660		Crippen Method
mcvol	156.900	ml/mol	McGowan Method
pc	3045.68	kPa	Joback Method
rinpol	1764.00		NIST Webbook
rinpol	1776.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1756.00		NIST Webbook
rinpol	1764.00		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	328.07	J/molxK	612.14	Joback Method
cpg	341.24	J/molxK	655.43	Joback Method
cpg	353.28	J/molxK	698.72	Joback Method
cpg	364.26	J/molxK	742.01	Joback Method
cpg	374.26	J/molxK	785.30	Joback Method
cpg	383.35	J/molxK	828.59	Joback Method
cpg	391.60	J/molxK	871.88	Joback Method
dvisc	0.0013975	Paxs	362.72	Joback Method
dvisc	0.0008516	Paxs	404.29	Joback Method
dvisc	0.0005691	Paxs	445.86	Joback Method
dvisc	0.0004074	Paxs	487.43	Joback Method
dvisc	0.0003074	Paxs	529.00	Joback Method
dvisc	0.0002417	Paxs	570.57	Joback Method
dvisc	0.0001963	Paxs	612.14	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	470.70	K	2.00	NIST Webbook

Sources

McGowan Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2974927&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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