1,1'-Biphenyl, 2,3',4,4',5-pentachloro-

Other names:	1,2,4-trichloro-5-(3,4-dichlorophenyl)benzene
	2,3',4,4',5-Pentachloro-1,1'-biphenyl
	2,3',4,4',5-Pentachlorobiphenyl
	2,4,5,3',4'-Pentachlorobiphenyl
	3,4,2',4',5'-Pentachlorobiphenyl
	Biphenyl, 2,3',4,4',5-pentachloro-
	PCB 118
Inchi:	InChI=1S/C12H5Cl5/c13-8-2-1-6(3-10(8)15)7-4-11(16)12(17)5-9(7)14/h1-5H
InchiKey:	IUTPYMGCWINGEY-UHFFFAOYSA-N
Formula:	C12H5Cl5
SMILES:	Clc1ccc(-c2cc(Cl)c(Cl)cc2Cl)cc1Cl
Mol. weight [g/mol]:	326.43
CAS:	31508-00-6

Physical Properties

Property code	Value	Unit	Source
gf	167.18	kJ/mol	Joback Method
hf	46.00	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	72.09	kJ/mol	Joback Method
log10ws	-7.39		Aqueous Solubility Prediction Method
logp	6.621		Crippen Method
mcvol	193.620	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	2291.00		NIST Webbook
rinpol	2276.00		NIST Webbook
rinpol	2277.00		NIST Webbook
rinpol	2278.90		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2278.90		NIST Webbook
tb	739.37	K	Joback Method
tc	1008.22	K	Joback Method
tf	490.04	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	428.46	J/mol×K	1008.22	Joback Method
cpg	423.09	J/mol×K	963.41	Joback Method
cpg	417.08	J/mol×K	918.60	Joback Method
cpg	410.38	J/mol×K	873.79	Joback Method
cpg	402.91	J/mol×K	828.99	Joback Method
cpg	394.64	J/mol×K	784.18	Joback Method
cpg	385.50	J/mol×K	739.37	Joback Method
dvisc	0.0006694	Pa×s	490.04	Joback Method
dvisc	0.0001570	Pa×s	739.37	Joback Method
dvisc	0.0001860	Pa×s	697.82	Joback Method
dvisc	0.0002252	Pa×s	656.26	Joback Method
dvisc	0.0002798	Pa×s	614.71	Joback Method
dvisc	0.0003588	Pa×s	573.15	Joback Method
dvisc	0.0004783	Pa×s	531.60	Joback Method
hvapt	89.30	kJ/mol	368.00	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/AqueousDa

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C31508006&Units=SI

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

Henry's Law Constants for Eleven Polychlorinated Biphenyls at 20 C: https://www.doi.org/10.1021/je0500835

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