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

Other names:	1,1'-Biphenyl, 2,2',3,4',5'-pentachloro-
	1,2,4-trichloro-5-(2,3-dichlorophenyl)benzene
	2,2',3',4,5-Pentachlorobiphenyl
	2,2',3',4,5-Pentachlorodiphenyl
	2,2',3,4,5-PCB
	2,4,5,2',3'-Pentachlorobiphenyl
	PCB-97
Inchi:	InChI=1S/C12H5Cl5/c13-8-3-1-2-6(12(8)17)7-4-10(15)11(16)5-9(7)14/h1-5H
InchiKey:	JTUSORDQZVOEAZ-UHFFFAOYSA-N
Formula:	C12H5Cl5
SMILES:	Clc1cc(Cl)c(-c2cccc(Cl)c2Cl)cc1Cl
Mol. weight [g/mol]:	326.44

Physical Properties

Property code	Value	Unit	Source
hf	66.29	kJ/mol	Cheméo Relay (1.0)
hfus	33.96	kJ/mol	Joback Method
hvap	97.81	kJ/mol	Cheméo Relay (1.0)
ie	8.47	eV	Cheméo Relay (1.0)
log10ws	-7.21		Aqueous Solubility Prediction Method
log10ws	-7.21		Estimated Solubility Method
logp	6.621		Crippen Method
mcvol	193.620	ml/mol	McGowan Method
rinpol	2159.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2175.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
tb	623.81	K	Cheméo Relay (1.0)
tf	360.11	K	Cheméo Relay (1.0)

Temperature Dependent Properties

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

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C41464511&Units=SI

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

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

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

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

hf: Enthalpy of formation at standard conditions

hfus: Enthalpy of fusion at standard conditions

hvap: Enthalpy of vaporization at standard conditions

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

Latest version available from:
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