

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]:	326.43
CAS:	41464-51-1

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	-7.21		Estimated Solubility Method
log10ws	-7.21		Aqueous Solubility Prediction Method
logp	6.621		Crippen Method
mcvol	193.620	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	2175.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2159.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2157.00		NIST Webbook
rinpol	2158.00		NIST Webbook
rinpol	2158.00		NIST Webbook
tb	739.37	K	Joback Method
tc	1008.22	K	Joback Method

tf	490.04	K	Joback Method
vc	0.737	m ³ /kmol	Joback Method

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	Paxs	490.04	Joback Method
dvisc	0.0004783	Paxs	531.60	Joback Method
dvisc	0.0003588	Paxs	573.15	Joback Method
dvisc	0.0002798	Paxs	614.71	Joback Method
dvisc	0.0002252	Paxs	656.26	Joback Method
dvisc	0.0001860	Paxs	697.82	Joback Method
dvisc	0.0001570	Paxs	739.37	Joback Method

Sources

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

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

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

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

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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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