

1,1'-Biphenyl, 2,2',3,4,6-Pentachloro-

Other names:	1,2,3,5-tetrachloro-4-(2-chlorophenyl)benzene 2,2',3,4,6-Pentachloro-1,1'-biphenyl 2,2',3,4,6-Pentachlorobiphenyl PCB 88
Inchi:	InChI=1S/C12H5Cl5/c13-7-4-2-1-3-6(7)10-8(14)5-9(15)11(16)12(10)17/h1-5H
InchiKey:	QGDKRLQRLFUJPP-UHFFFAOYSA-N
Formula:	C12H5Cl5
SMILES:	Clc1ccccc1-c1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	326.43
CAS:	55215-17-3

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	-7.43		Aqueous Solubility Prediction Method
logp	6.621		Crippen Method
mcvol	193.620	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
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	385.50	J/mol×K	739.37	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	428.46	J/mol×K	1008.22	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
dvisc	0.0006694	Pa×s	490.04	Joback Method

Sources

Joback Method:	https://en.wikipedia.org/wiki/Joback_method
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=C55215173&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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