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

Other names:	1,2,3,5-tetrachloro-4-(2,3,4-trichlorophenyl)benzene
	2,2',3,3',4,4',6-Heptachloro-1,1'-biphenyl
	2,2',3,3',4,4',6-Heptachlorobiphenyl
	2,3,3',4,4'6-PCB
	PCB 171
Inchi:	InChI=1S/C12H3Cl7/c13-5-2-1-4(9(16)10(5)17)8-6(14)3-7(15)11(18)12(8)19/h1-3H
InchiKey:	TZMHVHLTPWKZCI-UHFFFAOYSA-N
Formula:	C12H3Cl7
SMILES:	Clc1ccc(-c2c(Cl)cc(Cl)c(Cl)c2Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	395.32
CAS:	52663-71-5

Physical Properties

Property code	Value	Unit	Source
gf	124.06	kJ/mol	Joback Method
hf	-8.42	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	109.10	kJ/mol	NIST Webbook
log10ws	-8.30		Aqueous Solubility Prediction Method
log10ws	-7.66		Estimated Solubility Method
logp	7.927		Crippen Method
mcvol	218.100	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	2439.00		NIST Webbook
rinpol	2440.00		NIST Webbook
tb	824.19	K	Joback Method
tc	1096.84	K	Joback Method
tf	395.40 ± 0.20	K	NIST Webbook
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	415.14	J/mol×K	824.19	Joback Method
cpg	422.07	J/mol×K	869.63	Joback Method
cpg	428.26	J/mol×K	915.07	Joback Method
cpg	433.75	J/mol×K	960.51	Joback Method
cpg	438.58	J/mol×K	1005.96	Joback Method
cpg	442.79	J/mol×K	1051.40	Joback Method
cpg	446.42	J/mol×K	1096.84	Joback Method
dvisc	0.0004373	Pa×s	574.92	Joback Method
dvisc	0.0003321	Pa×s	616.47	Joback Method
dvisc	0.0002611	Pa×s	658.01	Joback Method
dvisc	0.0002113	Pa×s	699.56	Joback Method
dvisc	0.0001750	Pa×s	741.10	Joback Method
dvisc	0.0001479	Pa×s	782.64	Joback Method
dvisc	0.0001272	Pa×s	824.19	Joback Method
hvapt	95.90	kJ/mol	368.00	NIST Webbook

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=C52663715&Units=SI

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

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
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