1,1'-Biphenyl, 2,2',3,4,4',5,6-heptachloro-

Other names:	1,2,3,4,5-pentachloro-6-(2,4-dichlorophenyl)benzene
	2,2',3,4,4',5',6-PCB
	2,2',3,4,4',5,6-Heptachlorobiphenyl
	PCB 181
Inchi:	InChI=1S/C12H3Cl7/c13-4-1-2-5(6(14)3-4)7-8(15)10(17)12(19)11(18)9(7)16/h1-3H
InchiKey:	DJEUXBQAKBLKPO-UHFFFAOYSA-N
Formula:	C12H3Cl7
SMILES:	Clc1ccc(-c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c1
Mol. weight [g/mol]:	395.33

Physical Properties

Property code	Value	Unit	Source
hf	59.68	kJ/mol	Cheméo Relay (1.0)
hfus	41.57	kJ/mol	Joback Method
hvap	107.00	kJ/mol	Cheméo Relay (1.0)
ie	8.57	eV	Cheméo Relay (1.0)
log10ws	-7.92		Aqueous Solubility Prediction Method
log10ws	-7.92		Estimated Solubility Method
logp	7.927		Crippen Method
mcvol	218.100	ml/mol	McGowan Method
tb	657.66	K	Cheméo Relay (1.0)
tf	422.72	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.14	J/mol×K	824.19	Joback Method
cpg	446.42	J/mol×K	1096.84	Joback Method
cpg	442.79	J/mol×K	1051.40	Joback Method
cpg	438.58	J/mol×K	1005.96	Joback Method
cpg	433.75	J/mol×K	960.51	Joback Method
cpg	428.26	J/mol×K	915.07	Joback Method

cpg	422.07	J/mol×K	869.63	Joback Method
dvisc	0.0002113	Pa×s	699.56	Joback Method
dvisc	0.0001272	Pa×s	824.19	Joback Method
dvisc	0.0001479	Pa×s	782.64	Joback Method
dvisc	0.0001750	Pa×s	741.10	Joback Method
dvisc	0.0004373	Pa×s	574.92	Joback Method
dvisc	0.0002611	Pa×s	658.01	Joback Method
dvisc	0.0003321	Pa×s	616.47	Joback Method

Sources

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=C74472472&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

Cheméo Relay (1.0):

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
tb: Normal Boiling Point Temperature
tf: Normal melting (fusion) point