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

Other names:	1,2,3-trichloro-4-(2,4,5-trichlorophenyl)benzene
	2,2',3',4,4',5-Hexachlorobiphenyl
	2,2',3,4,4',5'-Hexachlorobiphenyl
	2,2',3,4,4',5'-hexachloro-1,1'-biphenyl
	2,3,4,2',4',5'-Hexachlorobiphenyl
	2,4,5,2',3',4'-hexachlorobiphenyl
	PCB-138
Inchi:	InChI=1S/C12H4Cl6/c13-7-2-1-5(11(17)12(7)18)6-3-9(15)10(16)4-8(6)14/h1-4H
InchiKey:	RPUMZMSNLZHIGZ-UHFFFAOYSA-N
Formula:	C12H4Cl6
SMILES:	Clc1cc(Cl)c(-c2ccc(Cl)c(Cl)c2Cl)cc1Cl
Mol. weight [g/mol]:	360.88
CAS:	35065-28-2

Physical Properties

Property code	Value	Unit	Source
gf	145.62	kJ/mol	Joback Method
hf	18.79	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	77.14	kJ/mol	Joback Method
log10ws	-8.32		Aqueous Solubility Prediction Method
logp	7.274		Crippen Method
mcvol	205.860	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2355.00		NIST Webbook
rinpol	2311.00		NIST Webbook
rinpol	2390.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2364.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2311.00		NIST Webbook
tb	781.78	K	Joback Method
tc	1052.68	K	Joback Method
tf	532.48	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	438.05	J/mol×K	1052.68	Joback Method
cpg	433.56	J/mol×K	1007.53	Joback Method
cpg	428.46	J/mol×K	962.38	Joback Method
cpg	422.71	J/mol×K	917.23	Joback Method
cpg	416.26	J/mol×K	872.08	Joback Method
cpg	409.07	J/mol×K	826.93	Joback Method
cpg	401.07	J/mol×K	781.78	Joback Method
dvisc	0.0005388	Pa×s	532.48	Joback Method
dvisc	0.0001419	Pa×s	781.78	Joback Method
dvisc	0.0001666	Pa×s	740.23	Joback Method
dvisc	0.0001992	Pa×s	698.68	Joback Method
dvisc	0.0002437	Pa×s	657.13	Joback Method
dvisc	0.0003063	Pa×s	615.58	Joback Method
dvisc	0.0003981	Pa×s	574.03	Joback Method
hvapt	91.90	kJ/mol	368.00	NIST Webbook

Sources

Henry's Law Constants for Eleven Polychlorinated Biphenyls at 20 C:	https://www.doi.org/10.1021/je0500835
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35065282&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
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