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

Other names:	1,2,3,4-tetrachloro-5-(3,4-dichlorophenyl)benzene
	2,3,3',4,4',5-HEXACHLORO-1,1'-BIPHENYL
	2,3,3',4,4',5-Hexachlorobiphenyl
	2,3,3',4,4',5-PCB
	2,3,4,4',5,5'-hexachlorobiphenyl
	2,3,4,5,3',4'-Hexachlorobiphenyl
	3,4,2',3',4',5'-Hexachlorobiphenyl
	PCB 156
Inchi:	InChI=1S/C12H4Cl6/c13-7-2-1-5(3-8(7)14)6-4-9(15)11(17)12(18)10(6)16/h1-4H
InchiKey:	LCXMEXLGMKFLQO-UHFFFAOYSA-N
Formula:	C12H4Cl6
SMILES:	Clc1ccc(-c2cc(Cl)c(Cl)c(Cl)c2Cl)cc1Cl
Mol. weight [g/mol]:	360.88
CAS:	38380-08-4

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	112.60 ± 0.40	kJ/mol	NIST Webbook
log10ws	-7.82		Estimated Solubility Method
log10ws	-7.82		Aqueous Solubility Prediction Method
logp	7.274		Crippen Method
mcvol	205.860	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2467.00		NIST Webbook
rinpol	2466.00		NIST Webbook
rinpol	2466.00		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	401.07	J/mol×K	781.78	Joback Method
cpg	409.07	J/mol×K	826.93	Joback Method
cpg	416.26	J/mol×K	872.08	Joback Method
cpg	422.71	J/mol×K	917.23	Joback Method
cpg	428.46	J/mol×K	962.38	Joback Method
cpg	433.56	J/mol×K	1007.53	Joback Method
cpg	438.05	J/mol×K	1052.68	Joback Method
dvisc	0.0005388	Pa×s	532.48	Joback Method
dvisc	0.0003981	Pa×s	574.03	Joback Method
dvisc	0.0003063	Pa×s	615.58	Joback Method
dvisc	0.0002437	Pa×s	657.13	Joback Method
dvisc	0.0001992	Pa×s	698.68	Joback Method
dvisc	0.0001666	Pa×s	740.23	Joback Method
dvisc	0.0001419	Pa×s	781.78	Joback Method
hvapt	94.80	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=C38380084&Units=SI

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

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

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