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

Other names:	1,2,3,4-tetrachloro-5-(2,3-dichlorophenyl)benzene
	2,2',3,3',4,5-Hexachloro-1,1'-biphenyl
	2,2',3,3',4,5-Hexachlorobiphenyl
	PCB 129
Inchi:	InChI=1S/C12H4Cl6/c13-7-3-1-2-5(9(7)15)6-4-8(14)11(17)12(18)10(6)16/h1-4H
InchiKey:	VQQKIXKPMJTUMP-UHFFFAOYSA-N
Formula:	C12H4Cl6
SMILES:	Clc1cccc(-c2cc(Cl)c(Cl)c(Cl)c2Cl)c1Cl
Mol. weight [g/mol]:	360.88
CAS:	55215-18-4

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	77.14	kJ/mol	Joback Method
log10ws	-8.56		Aqueous Solubility Prediction Method
logp	7.274		Crippen Method
mcvol	205.860	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2331.00		NIST Webbook
rinpol	2354.00		NIST Webbook
rinpol	2352.00		NIST Webbook
rinpol	2337.00		NIST Webbook
rinpol	2337.00		NIST Webbook
rinpol	2331.00		NIST Webbook
rinpol	2336.00		NIST Webbook
rinpol	2352.00		NIST Webbook
rinpol	2336.00		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	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	438.05	J/mol×K	1052.68	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
dvisc	0.0005388	Pa×s	532.48	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55215184&Units=SI

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

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

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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