2,3,3',4',5,6-Hexachloro-1,1'-biphenyl

Other names:	PCB 163
	1,1'-Biphenyl, 2,3,3',4',5,6-hexachloro
Inchi:	InChI=1S/C12H4Cl6/c13-6-2-1-5(3-7(6)14)10-11(17)8(15)4-9(16)12(10)18/h1-4H
InchiKey:	ZAGRQXMWMRUYRB-UHFFFAOYSA-N
Formula:	C12H4Cl6
SMILES:	Clc1ccc(-c2c(Cl)c(Cl)cc(Cl)c2Cl)cc1Cl
Mol. weight [g/mol]:	360.88
CAS:	74472-44-9

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	-8.18		Crippen Method
logp	7.274		Crippen Method
mcvol	205.860	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2348.00		NIST Webbook
rinpol	2370.00		NIST Webbook
rinpol	2348.00		NIST Webbook
rinpol	2367.00		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

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C74472449&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
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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