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

Other names:	2,2',3,3',4,5'-Hexachloro-1,1'-biphenyl
	1,1'-Biphenyl, 2,2',3,3',4',5-hexachloro
	PCB 130
Inchi:	InChI=1S/C12H4Cl6/c13-5-3-7(10(16)9(15)4-5)6-1-2-8(14)12(18)11(6)17/h1-4H
InchiKey:	YFSLABAYQDPWPF-UHFFFAOYSA-N
Formula:	C12H4Cl6
SMILES:	Clc1cc(Cl)c(Cl)c(-c2ccc(Cl)c(Cl)c2Cl)c1
Mol. weight [g/mol]:	360.88

Physical Properties

Property code	Value	Unit	Source
hf	43.95	kJ/mol	Cheméo Relay (1.0)
hfus	37.77	kJ/mol	Joback Method
hvap	104.26	kJ/mol	Cheméo Relay (1.0)
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-8.17		Cheméo Relay (1.0)
logp	7.274		Crippen Method
mcvol	205.860	ml/mol	McGowan Method
rinpol	2324.00		NIST Webbook
rinpol	2346.00		NIST Webbook
rinpol	2325.00		NIST Webbook
rinpol	2325.00		NIST Webbook
tb	642.91	K	Cheméo Relay (1.0)
tf	368.77	K	Cheméo Relay (1.0)

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
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52663668&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

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

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