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

Other names:	PCB 161
	1,1'-Biphenyl, 2,3,3',4,5',6-hexachloro
Inchi:	InChI=1S/C12H4Cl6/c13-6-1-5(2-7(14)3-6)10-8(15)4-9(16)11(17)12(10)18/h1-4H
InchiKey:	UNPTZXSJGZTGJJ-UHFFFAOYSA-N
Formula:	C12H4Cl6
SMILES:	Clc1cc(Cl)cc(-c2c(Cl)cc(Cl)c(Cl)c2Cl)c1
Mol. weight [g/mol]:	360.88
CAS:	74472-43-8

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	2336.00		NIST Webbook
rinpol	2338.00		NIST Webbook
rinpol	2337.00		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

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=C74472438&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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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