1,1'-Biphenyl, 2,2',3,3',5-pentachloro-

Other names:	2,2',3,3',5-Pentachloro-1,1'-biphenyl
	PCB 83
Inchi:	InChI=1S/C12H5Cl5/c13-6-4-8(12(17)10(15)5-6)7-2-1-3-9(14)11(7)16/h1-5H
InchiKey:	SUBRHHYLRGOTHL-UHFFFAOYSA-N
Formula:	C12H5Cl5
SMILES:	Clc1cc(Cl)c(Cl)c(-c2cccc(Cl)c2Cl)c1
Mol. weight [g/mol]:	326.43
CAS:	60145-20-2

Physical Properties

Property code	Value	Unit	Source
gf	167.18	kJ/mol	Joback Method
hf	46.00	kJ/mol	Joback Method
hfus	33.96	kJ/mol	Joback Method
hvap	72.09	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	6.621		Crippen Method
mcvol	193.620	ml/mol	McGowan Method
pc	2581.96	kPa	Joback Method
rinpol	2139.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2140.00		NIST Webbook
rinpol	2136.00		NIST Webbook
rinpol	2087.00		NIST Webbook
rinpol	2139.00		NIST Webbook
tb	739.37	K	Joback Method
tc	1008.22	K	Joback Method
tf	490.04	K	Joback Method
vc	0.737	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.50	J/mol×K	739.37	Joback Method

cpg	423.09	J/mol×K	963.41	Joback Method
cpg	417.08	J/mol×K	918.60	Joback Method
cpg	410.38	J/mol×K	873.79	Joback Method
cpg	402.91	J/mol×K	828.99	Joback Method
cpg	394.64	J/mol×K	784.18	Joback Method
cpg	428.46	J/mol×K	1008.22	Joback Method
dvisc	0.0001570	Pa×s	739.37	Joback Method
dvisc	0.0001860	Pa×s	697.82	Joback Method
dvisc	0.0002252	Pa×s	656.26	Joback Method
dvisc	0.0002798	Pa×s	614.71	Joback Method
dvisc	0.0003588	Pa×s	573.15	Joback Method
dvisc	0.0004783	Pa×s	531.60	Joback Method
dvisc	0.0006694	Pa×s	490.04	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C60145202&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
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
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