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

Other names:	2,2',3,3',4,5,5'-Heptachloro-1,1'-biphenyl
	1,1'-Biphenyl, 2,2',3,3',4',5,5'-heptachloro
	PCB 172
Inchi:	InChI=1S/C12H3Cl7/c13-4-1-5(9(16)7(14)2-4)6-3-8(15)11(18)12(19)10(6)17/h1-3H
InchiKey:	HOPMUCXYRNOABF-UHFFFAOYSA-N
Formula:	C12H3Cl7
SMILES:	Clc1cc(Cl)c(Cl)c(-c2cc(Cl)c(Cl)c(Cl)c2Cl)c1
Mol. weight [g/mol]:	395.32
CAS:	52663-74-8

Physical Properties

Property code	Value	Unit	Source
gf	124.06	kJ/mol	Joback Method
hf	-8.42	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	7.927		Crippen Method
mcvol	218.100	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	2477.00		NIST Webbook
rinpol	2476.00		NIST Webbook
tb	824.19	K	Joback Method
tc	1096.84	K	Joback Method
tf	574.92	K	Joback Method
vc	0.835	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.14	J/mol×K	824.19	Joback Method
cpg	422.07	J/mol×K	869.63	Joback Method
cpg	428.26	J/mol×K	915.07	Joback Method
cpg	433.75	J/mol×K	960.51	Joback Method

cpg	438.58	J/mol×K	1005.96	Joback Method
cpg	442.79	J/mol×K	1051.40	Joback Method
cpg	446.42	J/mol×K	1096.84	Joback Method
dvisc	0.0004373	Pa×s	574.92	Joback Method
dvisc	0.0003321	Pa×s	616.47	Joback Method
dvisc	0.0002611	Pa×s	658.01	Joback Method
dvisc	0.0002113	Pa×s	699.56	Joback Method
dvisc	0.0001750	Pa×s	741.10	Joback Method
dvisc	0.0001479	Pa×s	782.64	Joback Method
dvisc	0.0001272	Pa×s	824.19	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52663748&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

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