1,1'-Biphenyl, 2,2',3,3',5,5',6-heptachloro-

Other names:	2,2',3,3',5,5',6-Heptachloro-1,1'-biphenyl
	PCB 178
	2,2',3,3',5,5',6-Heptachlorobiphenyl
Inchi:	InChI=1S/C12H3Cl7/c13-4-1-5(10(17)6(14)2-4)9-11(18)7(15)3-8(16)12(9)19/h1-3H
InchiKey:	WCIBKXHMIXUQHK-UHFFFAOYSA-N
Formula:	C12H3Cl7
SMILES:	Clc1cc(Cl)c(Cl)c(-c2c(Cl)c(Cl)cc(Cl)c2Cl)c1
Mol. weight [g/mol]:	395.32
CAS:	52663-67-9

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	2364.00		NIST Webbook
rinpol	2332.00		NIST Webbook
rinpol	2359.00		NIST Webbook
rinpol	2364.00		NIST Webbook
rinpol	2361.00		NIST Webbook
rinpol	2332.00		NIST Webbook
rinpol	2361.00		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	446.42	J/mol×K	1096.84	Joback Method
cpg	442.79	J/mol×K	1051.40	Joback Method
cpg	438.58	J/mol×K	1005.96	Joback Method
cpg	433.75	J/mol×K	960.51	Joback Method
cpg	428.26	J/mol×K	915.07	Joback Method
cpg	422.07	J/mol×K	869.63	Joback Method
cpg	415.14	J/mol×K	824.19	Joback Method
dvisc	0.0004373	Pa×s	574.92	Joback Method
dvisc	0.0001272	Pa×s	824.19	Joback Method
dvisc	0.0001479	Pa×s	782.64	Joback Method
dvisc	0.0001750	Pa×s	741.10	Joback Method
dvisc	0.0002113	Pa×s	699.56	Joback Method
dvisc	0.0002611	Pa×s	658.01	Joback Method
dvisc	0.0003321	Pa×s	616.47	Joback Method
hfust	20.30	kJ/mol	395.40	NIST Webbook

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=C52663679&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
hfust: Enthalpy of fusion at a given temperature
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