1,1'-Biphenyl, 2,2',4,6-tetrachloro-

Other names: 2,2',4,6-Tetrachloro-1,1'-biphenyl
2,2',4,6-Tetrachlorobiphenyl
PCB 50
Inchi: InChI=1S/C12H6Cl4/c13-7-5-10(15)12(11(16)6-7)8-3-1-2-4-9(8)14/h1-6H
InchiKey: VLLVVZDKBSYMCG-UHFFFAOYSA-N
Formula: C12H6Cl4
SMILES: Clc1cc(Cl)c(-c2ccccc2Cl)c(Cl)c1
Mol. weight [g/mol]: 291.99

Physical Properties

Property code	Value	Unit	Source
af	0.4853		Cheméo Relay (1.0)
gf	188.74	kJ/mol	Joback Method
hf	110.78	kJ/mol	Cheméo Relay (1.0)
hfus	30.15	kJ/mol	Joback Method
hvap	84.24	kJ/mol	Cheméo Relay (1.0)
ie	8.52	eV	Cheméo Relay (1.0)
log10ws	-6.63		Cheméo Relay (1.0)
logp	5.967		Crippen Method
mcvol	181.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1831.00		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	1835.00		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1831.00		NIST Webbook
rinpol	1873.00		NIST Webbook
tb	595.26	K	Cheméo Relay (1.0)
tc	877.28	K	Cheméo Relay (1.0)
tf	337.48	K	Cheméo Relay (1.0)
vc	0.652	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	368.27	J/mol×K	696.96	Joback Method
cpg	378.65	J/mol×K	741.36	Joback Method
cpg	388.08	J/mol×K	785.76	Joback Method
cpg	396.63	J/mol×K	830.15	Joback Method
cpg	404.36	J/mol×K	874.55	Joback Method
cpg	411.33	J/mol×K	918.95	Joback Method
cpg	417.60	J/mol×K	963.35	Joback Method
dvisc	0.0008409	Pa×s	447.60	Joback Method
dvisc	0.0005766	Pa×s	489.16	Joback Method
dvisc	0.0004195	Pa×s	530.72	Joback Method
dvisc	0.0003196	Pa×s	572.28	Joback Method
dvisc	0.0002526	Pa×s	613.84	Joback Method
dvisc	0.0002057	Pa×s	655.40	Joback Method
dvisc	0.0001717	Pa×s	696.96	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C62796650&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

af: Acentric Factor
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
ie: Ionization energy
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