1,1'-Biphenyl, 2,2',4,4',5-pentachloro-

Other names: 2,2',4,4'5-Pentachlorobiphenyl
2,2',4,4',5-Pentachloro-1,1'-biphenyl
PCB 99
Inchi: InChI=1S/C12H5Cl5/c13-6-1-2-7(9(14)3-6)8-4-11(16)12(17)5-10(8)15/h1-5H
InchiKey: LMQJBFRGXHMNOX-UHFFFAOYSA-N
Formula: C12H5Cl5
SMILES: Clc1ccc(-c2cc(Cl)c(Cl)cc2Cl)c(Cl)c1
Mol. weight [g/mol]: 326.43
CAS: 38380-01-7

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	2150.00		NIST Webbook
rinpol	2151.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2150.00		NIST Webbook
rinpol	2150.00		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	428.46	J/mol×K	1008.22	Joback Method

cpg	385.50	J/mol×K	739.37	Joback Method
cpg	394.64	J/mol×K	784.18	Joback Method
cpg	402.91	J/mol×K	828.99	Joback Method
cpg	410.38	J/mol×K	873.79	Joback Method
cpg	417.08	J/mol×K	918.60	Joback Method
cpg	423.09	J/mol×K	963.41	Joback Method
dvisc	0.0001570	Pa×s	739.37	Joback Method
dvisc	0.0006694	Pa×s	490.04	Joback Method
dvisc	0.0004783	Pa×s	531.60	Joback Method
dvisc	0.0003588	Pa×s	573.15	Joback Method
dvisc	0.0002798	Pa×s	614.71	Joback Method
dvisc	0.0002252	Pa×s	656.26	Joback Method
dvisc	0.0001860	Pa×s	697.82	Joback Method
hvapt	86.80	kJ/mol	368.00	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=C38380017&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
hvapt:	Enthalpy of vaporization at a given temperature
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