2,3',4,5-Tetrachloro-1,1'-biphenyl

Other names:	1,1'-Biphenyl, 2,3',4,5-tetrachloro
	PCB 67
Inchi:	InChI=1S/C12H6Cl4/c13-8-3-1-2-7(4-8)9-5-11(15)12(16)6-10(9)14/h1-6H
InchiKey:	LQEGJNOKOZHBBZ-UHFFFAOYSA-N
Formula:	C12H6Cl4
SMILES:	Clc1cccc(-c2cc(Cl)c(Cl)cc2Cl)c1
Mol. weight [g/mol]:	291.99
CAS:	73575-53-8

Physical Properties

Property code	Value	Unit	Source
gf	188.74	kJ/mol	Joback Method
hf	73.21	kJ/mol	Joback Method
hfus	30.15	kJ/mol	Joback Method
hvap	67.05	kJ/mol	Joback Method
log10ws	-6.81		Crippen Method
logp	5.967		Crippen Method
mcvol	181.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1968.00		NIST Webbook
rinpol	1967.00		NIST Webbook
tb	696.96	K	Joback Method
tc	963.35	K	Joback Method
tf	447.60	K	Joback Method
vc	0.688	m3/kmol	Joback Method

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

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=C73575538&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
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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