

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

Other names:	2,2',4,4'-Tetrachloro-1,1'-biphenyl 2,2',4,4'-Tetrachlorobiphenyl 2,2',4,4'-Tetrachlorodiphenyl 2,4-dichloro-1-(2,4-dichlorophenyl)benzene Biphenyl, 2,2',4,4'-tetrachloro- PCB 47
Inchi:	InChI=1S/C12H6Cl4/c13-7-1-3-9(11(15)5-7)10-4-2-8(14)6-12(10)16/h1-6H
InchiKey:	QORAVNMWUNPXAO-UHFFFAOYSA-N
Formula:	C12H6Cl4
SMILES:	Clc1ccc(-c2ccc(Cl)cc2Cl)c(Cl)c1
Mol. weight [g/mol]:	291.99
CAS:	2437-79-8

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	-6.51		Aqueous Solubility Prediction Method
logp	5.967		Crippen Method
mcvol	181.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1951.00		NIST Webbook
rinpol	1913.60		NIST Webbook
rinpol	1914.00		NIST Webbook
rinpol	1986.00		NIST Webbook
rinpol	1986.00		NIST Webbook
rinpol	1937.10		NIST Webbook
rinpol	1917.20		NIST Webbook
rinpol	1927.30		NIST Webbook
rinpol	1937.60		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/molxK	696.96	Joback Method
cpg	411.33	J/molxK	918.95	Joback Method
cpg	404.36	J/molxK	874.55	Joback Method
cpg	396.63	J/molxK	830.15	Joback Method
cpg	388.08	J/molxK	785.76	Joback Method
cpg	378.65	J/molxK	741.36	Joback Method
cpg	417.60	J/molxK	963.35	Joback Method
dvisc	0.0001717	Paxs	696.96	Joback Method
dvisc	0.0002057	Paxs	655.40	Joback Method
dvisc	0.0002526	Paxs	613.84	Joback Method
dvisc	0.0003196	Paxs	572.28	Joback Method
dvisc	0.0004195	Paxs	530.72	Joback Method
dvisc	0.0005766	Paxs	489.16	Joback Method
dvisc	0.0008409	Paxs	447.60	Joback Method

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Joback Method:

https://en.wikipedia.org/wiki/Joback_method

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2437798&Units=SI>

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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