

2,2',3,6-Tetrachloro-1,1'-biphenyl

Other names:	PCB 45 1,1'-Biphenyl, 2,2',3,6-tetrachloro-
Inchi:	InChI=1S/C12H6Cl4/c13-8-4-2-1-3-7(8)11-9(14)5-6-10(15)12(11)16/h1-6H
InchiKey:	VHGHZZTMJLTJX-UHFFFAOYSA-N
Formula:	C12H6Cl4
SMILES:	Clc1ccccc1-c1c(Cl)ccc(Cl)c1Cl
Mol. weight [g/mol]:	291.99
CAS:	70362-45-7

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
mvol	181.380	ml/mol	McGowan Method
pc	2724.01	kPa	Joback Method
rinpol	1851.00		NIST Webbook
rinpol	1851.00		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/molxK	696.96	Joback Method
cpg	378.65	J/molxK	741.36	Joback Method
cpg	388.08	J/molxK	785.76	Joback Method
cpg	396.63	J/molxK	830.15	Joback Method
cpg	404.36	J/molxK	874.55	Joback Method

cpg	411.33	J/molxK	918.95	Joback Method
cpg	417.60	J/molxK	963.35	Joback Method
dvisc	0.0008409	Paxs	447.60	Joback Method
dvisc	0.0005766	Paxs	489.16	Joback Method
dvisc	0.0004195	Paxs	530.72	Joback Method
dvisc	0.0003196	Paxs	572.28	Joback Method
dvisc	0.0002526	Paxs	613.84	Joback Method
dvisc	0.0002057	Paxs	655.40	Joback Method
dvisc	0.0001717	Paxs	696.96	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C70362457&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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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