

1,1'-Biphenyl, 2,2',3,3',4,4',5,5',6-nonachloro-

Other names:	1,2,3,4,5-pentachloro-6-(2,3,4,5-tetrachlorophenyl)benzene 2,2',3,3',4,4',5,5',6-Nonachloro-1,1'-biphenyl 2,2',3,3',4,4',5,5',6-Nonachlorobiphenyl 2,3,4,5,6,2',3',4',5'-Nonachlorobiphenyl Biphenyl, 2,2',3,3',4,4',5,5',6-nonachloro- PCB 206
Inchi:	InChI=1S/C12HCl9/c13-3-1-2(5(14)9(18)6(3)15)4-7(16)10(19)12(21)11(20)8(4)17/h1H
InchiKey:	JFIMDKGRGPNPRQ-UHFFFAOYSA-N
Formula:	C12HCl9
SMILES:	Clc1cc(-c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	464.21
CAS:	40186-72-9

Physical Properties

Property code	Value	Unit	Source
gf	80.94	kJ/mol	Joback Method
hf	-62.84	kJ/mol	Joback Method
hfus	49.19	kJ/mol	Joback Method
hvap	92.28	kJ/mol	Joback Method
log10ws	-10.26		Aqueous Solubility Prediction Method
logp	9.234		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2753.40		NIST Webbook
rinpol	2721.00		NIST Webbook
rinpol	2786.00		NIST Webbook
rinpol	2753.40		NIST Webbook
rinpol	2721.00		NIST Webbook
tb	909.01	K	Joback Method
tc	1184.69	K	Joback Method
tf	659.80	K	Joback Method
vc	0.932	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	439.23	J/mol×K	909.01	Joback Method
cpg	457.66	J/mol×K	1138.74	Joback Method
cpg	455.22	J/mol×K	1092.79	Joback Method
cpg	452.18	J/mol×K	1046.85	Joback Method
cpg	448.52	J/mol×K	1000.90	Joback Method
cpg	444.21	J/mol×K	954.96	Joback Method
cpg	459.52	J/mol×K	1184.69	Joback Method
dvisc	0.0000999	Pa×s	909.01	Joback Method
dvisc	0.0001145	Pa×s	867.48	Joback Method
dvisc	0.0001331	Pa×s	825.94	Joback Method
dvisc	0.0001571	Pa×s	784.40	Joback Method
dvisc	0.0001889	Pa×s	742.87	Joback Method
dvisc	0.0002322	Pa×s	701.34	Joback Method
dvisc	0.0002929	Pa×s	659.80	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C40186729&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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