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

Other names: 1,2,3,4,5-pentachloro-6-(2,3,5,6-tetrachlorophenyl)benzene
2,2',3,3',4,5,5',6,6'-Nonachlorobiphenyl
PCB 208
Inchi: InChI=1S/C12HCl9/c13-2-1-3(14)7(16)4(6(2)15)5-8(17)10(19)12(21)11(20)9(5)18/h1H
InchiKey: XIFFTDRFWYFAPO-UHFFFAOYSA-N
Formula: C12HCl9
SMILES: Clc1cc(Cl)c(Cl)c(-c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)c1Cl
Mol. weight [g/mol]: 464.21
CAS: 52663-77-1

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	-10.41		Aqueous Solubility Prediction Method
logp	9.234		Crippen Method
mcvol	242.580	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	2597.00		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	444.21	J/mol×K	954.96	Joback Method
cpg	448.52	J/mol×K	1000.90	Joback Method
cpg	452.18	J/mol×K	1046.85	Joback Method

cpg	455.22	J/mol×K	1092.79	Joback Method
cpg	457.66	J/mol×K	1138.74	Joback Method
cpg	459.52	J/mol×K	1184.69	Joback Method
dvisc	0.0002929	Pa×s	659.80	Joback Method
dvisc	0.0002322	Pa×s	701.34	Joback Method
dvisc	0.0001889	Pa×s	742.87	Joback Method
dvisc	0.0001571	Pa×s	784.40	Joback Method
dvisc	0.0001331	Pa×s	825.94	Joback Method
dvisc	0.0001145	Pa×s	867.48	Joback Method
dvisc	0.0000999	Pa×s	909.01	Joback Method
hfust	22.60	kJ/mol	455.80	NIST Webbook

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/AqueousDa

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C52663771&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

hfust: Enthalpy of fusion at a given temperature

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