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

Other names: 2,2',3,4,5,6'-Hexachloro-1,1'-biphenyl
2,2',3,4,5,6'-Hexachlorobiphenyl
PCB 143
Inchi: InChI=1S/C12H4Cl6/c13-6-2-1-3-7(14)9(6)5-4-8(15)11(17)12(18)10(5)16/h1-4H
InchiKey: UQPQKLGBEKEZBV-UHFFFAOYSA-N
Formula: C12H4Cl6
SMILES: Clc1cc(-c2c(Cl)cccc2Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 360.88
CAS: 68194-15-0

Physical Properties

Property code	Value	Unit	Source
gf	145.62	kJ/mol	Joback Method
hf	18.79	kJ/mol	Joback Method
hfus	37.77	kJ/mol	Joback Method
hvap	77.14	kJ/mol	Joback Method
log10ws	-8.18		Crippen Method
logp	7.274		Crippen Method
mcvol	205.860	ml/mol	McGowan Method
pc	2450.74	kPa	Joback Method
rinpol	2252.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2250.00		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	2250.00		NIST Webbook
tb	781.78	K	Joback Method
tc	1052.68	K	Joback Method
tf	532.48	K	Joback Method
vc	0.785	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	401.07	J/mol×K	781.78	Joback Method

cpg	409.07	J/mol×K	826.93	Joback Method
cpg	416.26	J/mol×K	872.08	Joback Method
cpg	422.71	J/mol×K	917.23	Joback Method
cpg	428.46	J/mol×K	962.38	Joback Method
cpg	433.56	J/mol×K	1007.53	Joback Method
cpg	438.05	J/mol×K	1052.68	Joback Method
dvisc	0.0005388	Pa×s	532.48	Joback Method
dvisc	0.0003981	Pa×s	574.03	Joback Method
dvisc	0.0003063	Pa×s	615.58	Joback Method
dvisc	0.0002437	Pa×s	657.13	Joback Method
dvisc	0.0001992	Pa×s	698.68	Joback Method
dvisc	0.0001666	Pa×s	740.23	Joback Method
dvisc	0.0001419	Pa×s	781.78	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

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=C68194150&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