

2,3,3',4,5,5'-Hexachloro-1,1'-biphenyl

Other names:	PCB 159 1,1'-Biphenyl, 2,3,3',4,5,5'-hexachloro
Inchi:	InChI=1S/C12H4Cl6/c13-6-1-5(2-7(14)3-6)8-4-9(15)11(17)12(18)10(8)16/h1-4H
InchiKey:	YZKLGRAIIIIGOHB-UHFFFAOYSA-N
Formula:	C12H4Cl6
SMILES:	Clc1cc(Cl)cc(-c2cc(Cl)c(Cl)c(Cl)c2Cl)c1
Mol. weight [g/mol]:	360.88
CAS:	39635-35-3

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	2344.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2300.00		NIST Webbook
rinpol	2301.00		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/molxK	781.78	Joback Method
cpg	409.07	J/molxK	826.93	Joback Method
cpg	416.26	J/molxK	872.08	Joback Method

cpg	422.71	J/molxK	917.23	Joback Method
cpg	428.46	J/molxK	962.38	Joback Method
cpg	433.56	J/molxK	1007.53	Joback Method
cpg	438.05	J/molxK	1052.68	Joback Method
dvisc	0.0005388	Paxs	532.48	Joback Method
dvisc	0.0003981	Paxs	574.03	Joback Method
dvisc	0.0003063	Paxs	615.58	Joback Method
dvisc	0.0002437	Paxs	657.13	Joback Method
dvisc	0.0001992	Paxs	698.68	Joback Method
dvisc	0.0001666	Paxs	740.23	Joback Method
dvisc	0.0001419	Paxs	781.78	Joback Method

Sources

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=C39635353&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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