

1,1'-Biphenyl, 2,2',4,4',5',6-hexachloro-

Other names:	2,2',4,4',5,6'-Hexachloro-1,1'-biphenyl 2,2',4,4',5,6'-Hexachlorobiphenyl PCB 154 1,1'-Biphenyl, 2,2',4,4',5,6'-hexachloro
Inchi:	InChI=1S/C12H4Cl6/c13-5-1-10(17)12(11(18)2-5)6-3-8(15)9(16)4-7(6)14/h1-4H
InchiKey:	QXZHEJWDLVUFFB-UHFFFAOYSA-N
Formula:	C12H4Cl6
SMILES:	Clc1cc(Cl)c(-c2cc(Cl)c(Cl)cc2Cl)c(Cl)c1
Mol. weight [g/mol]:	360.88

Physical Properties

Property code	Value	Unit	Source
hf	48.49	kJ/mol	Cheméo Relay (1.0)
hfus	37.77	kJ/mol	Joback Method
hvap	99.73	kJ/mol	Cheméo Relay (1.0)
ie	8.61	eV	Cheméo Relay (1.0)
log10ws	-8.14		Cheméo Relay (1.0)
logp	7.274		Crippen Method
mcvol	205.860	ml/mol	McGowan Method
tb	614.64	K	Cheméo Relay (1.0)
tf	373.81	K	Cheméo Relay (1.0)

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:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60145224&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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