

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

Other names:	PCB 182
Inchi:	InChI=1S/C12H3Cl7/c13-4-1-6(14)9(7(15)2-4)5-3-8(16)11(18)12(19)10(5)17/h1-3H
InchiKey:	RXRLRYZUMSYVLS-UHFFFAOYSA-N
Formula:	C12H3Cl7
SMILES:	Clc1cc(Cl)c(-c2cc(Cl)c(Cl)c(Cl)c2Cl)c(Cl)c1
Mol. weight [g/mol]:	395.33

Physical Properties

Property code	Value	Unit	Source
hf	39.23	kJ/mol	Cheméo Relay (1.0)
hfus	41.57	kJ/mol	Joback Method
hvap	105.59	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-8.87		Cheméo Relay (1.0)
logp	7.927		Crippen Method
mcvol	218.100	ml/mol	McGowan Method
rinpol	2402.00		NIST Webbook
rinpol	2402.00		NIST Webbook
tb	640.87	K	Cheméo Relay (1.0)
tf	395.01	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.14	J/mol×K	824.19	Joback Method
cpg	422.07	J/mol×K	869.63	Joback Method
cpg	428.26	J/mol×K	915.07	Joback Method
cpg	433.75	J/mol×K	960.51	Joback Method
cpg	438.58	J/mol×K	1005.96	Joback Method
cpg	442.79	J/mol×K	1051.40	Joback Method
cpg	446.42	J/mol×K	1096.84	Joback Method
dvisc	0.0004373	Pa×s	574.92	Joback Method
dvisc	0.0003321	Pa×s	616.47	Joback Method
dvisc	0.0002611	Pa×s	658.01	Joback Method

dvisc	0.0002113	Pa×s	699.56	Joback Method
dvisc	0.0001750	Pa×s	741.10	Joback Method
dvisc	0.0001479	Pa×s	782.64	Joback Method
dvisc	0.0001272	Pa×s	824.19	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C60145235&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>

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

Cheméo Relay (1.0):

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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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<https://www.chemeo.com/cid/21-515-6/1-1-Biphenyl-2-2-3-4-4-5-6-heptachloro.pdf>

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