

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

Other names:	2,2',3,4,4',5,5'-heptachloro-1,1'-biphenyl 2,2',3,4,4',5,5'-heptachlorobiphenyl 2,3,4,5,2',4',5'-heptachlorobiphenyl PCB 180
Inchi:	InChI=1S/C12H3Cl7/c13-6-3-8(15)7(14)1-4(6)5-2-9(16)11(18)12(19)10(5)17/h1-3H
InchiKey:	WBHQEUPUMONIKF-UHFFFAOYSA-N
Formula:	C12H3Cl7
SMILES:	Clc1cc(Cl)c(-c2cc(Cl)c(Cl)c(Cl)c2Cl)cc1Cl
Mol. weight [g/mol]:	395.32
CAS:	35065-29-3

Physical Properties

Property code	Value	Unit	Source
gf	124.06	kJ/mol	Joback Method
hf	-8.42	kJ/mol	Joback Method
hfus	41.57	kJ/mol	Joback Method
hvap	82.19	kJ/mol	Joback Method
log10ws	-8.87		Crippen Method
logp	7.927		Crippen Method
mcvol	218.100	ml/mol	McGowan Method
pc	2329.27	kPa	Joback Method
rinpol	2473.10		NIST Webbook
rinpol	2473.10		NIST Webbook
rinpol	2526.00		NIST Webbook
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	824.19	K	Joback Method
tc	1096.84	K	Joback Method
tf	574.92	K	Joback Method
vc	0.835	m3/kmol	Joback Method

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	Paxs	574.92	Joback Method
dvisc	0.0003321	Paxs	616.47	Joback Method
dvisc	0.0002611	Paxs	658.01	Joback Method
dvisc	0.0002113	Paxs	699.56	Joback Method
dvisc	0.0001750	Paxs	741.10	Joback Method
dvisc	0.0001479	Paxs	782.64	Joback Method
dvisc	0.0001272	Paxs	824.19	Joback Method
hvapt	96.50	kJ/mol	368.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C35065293&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Henry's Law Constants for Eleven Polychlorinated Biphenyls at 20 C:	https://www.doi.org/10.1021/je0500835
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
hvapt:	Enthalpy of vaporization at a given temperature
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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