2,2',3,4,4',5,5'-Heptachlorobiphenyl

Other names: 1,1'-biphenyl, 2,2',3,4,4',5,5'-heptachloro-
2,2',3,4,4',5,5'-heptachloro-1,1'-biphenyl
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]: 395.33

Physical Properties

Property code	Value	Unit	Source
hf	25.08	kJ/mol	Cheméo Relay (1.0)
hfus	41.57	kJ/mol	Joback Method
hvap	112.63	kJ/mol	Cheméo Relay (1.0)
ie	8.56	eV	Cheméo Relay (1.0)
log10ws	-8.90		Cheméo Relay (1.0)
logp	7.927		Crippen Method
mcvol	218.100	ml/mol	McGowan Method
rinpol	2494.00		NIST Webbook
rinpol	2473.10		NIST Webbook
rinpol	2473.10		NIST Webbook
rinpol	2494.00		NIST Webbook
rinpol	2526.00		NIST Webbook
rinpol	2494.00		NIST Webbook
tb	650.57	K	Cheméo Relay (1.0)
tf	402.41	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	446.42	J/mol×K	1096.84	Joback Method
cpg	442.79	J/mol×K	1051.40	Joback Method

cpg	438.58	J/mol×K	1005.96	Joback Method
cpg	433.75	J/mol×K	960.51	Joback Method
cpg	428.26	J/mol×K	915.07	Joback Method
cpg	422.07	J/mol×K	869.63	Joback Method
dvisc	0.0002113	Pa×s	699.56	Joback Method
dvisc	0.0001272	Pa×s	824.19	Joback Method
dvisc	0.0001479	Pa×s	782.64	Joback Method
dvisc	0.0001750	Pa×s	741.10	Joback Method
dvisc	0.0004373	Pa×s	574.92	Joback Method
dvisc	0.0002611	Pa×s	658.01	Joback Method
dvisc	0.0003321	Pa×s	616.47	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
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):	
Cheméo Relay (1.0, beta):	
Henry's Law Constants for Eleven Polychlorinated Biphenyls at 20 C:	https://www.doi.org/10.1021/je0500835

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
hvapt:	Enthalpy of vaporization at a given temperature
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