

2,2',3,4',5,6,6'-Heptachloro-1,1'-biphenyl

Other names:	PCB 188 1,1'-Biphenyl, 2,2',3,4',5,6,6'-heptachloro
Inchi:	InChI=1S/C12H3Cl7/c13-4-1-5(14)9(6(15)2-4)10-11(18)7(16)3-8(17)12(10)19/h1-3H
InchiKey:	MMTJWDQKGUNSDK-UHFFFAOYSA-N
Formula:	C12H3Cl7
SMILES:	Clc1cc(Cl)c(-c2c(Cl)c(Cl)cc(Cl)c2Cl)c(Cl)c1
Mol. weight [g/mol]:	395.32
CAS:	74487-85-7

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
rinpola	2275.00		NIST Webbook
tb	824.19	K	Joback Method
tc	1096.84	K	Joback Method
tf	574.92	K	Joback Method
vc	0.835	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.14	J/molxK	824.19	Joback Method
cpg	442.79	J/molxK	1051.40	Joback Method
cpg	438.58	J/molxK	1005.96	Joback Method
cpg	433.75	J/molxK	960.51	Joback Method
cpg	428.26	J/molxK	915.07	Joback Method
cpg	422.07	J/molxK	869.63	Joback Method

cpg	446.42	J/molxK	1096.84	Joback Method
dvisc	0.0001272	Paxs	824.19	Joback Method
dvisc	0.0001479	Paxs	782.64	Joback Method
dvisc	0.0001750	Paxs	741.10	Joback Method
dvisc	0.0002113	Paxs	699.56	Joback Method
dvisc	0.0002611	Paxs	658.01	Joback Method
dvisc	0.0003321	Paxs	616.47	Joback Method
dvisc	0.0004373	Paxs	574.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=C74487857&Units=SI

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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