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

Other names: 2,3,4,4',5-Pentachlorobiphenyl
PCB 114
Inchi: InChI=1S/C12H5Cl5/c13-7-3-1-6(2-4-7)8-5-9(14)11(16)12(17)10(8)15/h1-5H
InchiKey: SXZSFWHOSHAKMN-UHFFFAOYSA-N
Formula: C12H5Cl5
SMILES: Clc1ccc(-c2cc(Cl)c(Cl)c(Cl)c2Cl)cc1
Mol. weight [g/mol]: 326.44

Physical Properties

Property code	Value	Unit	Source
hf	79.34	kJ/mol	Cheméo Relay (1.0)
hfus	33.96	kJ/mol	Joback Method
hvap	100.05	kJ/mol	Cheméo Relay (1.0)
ie	8.41	eV	Cheméo Relay (1.0)
log10ws	-7.74		Cheméo Relay (1.0)
logp	6.621		Crippen Method
mcvol	193.620	ml/mol	McGowan Method
rinpol	2304.60		NIST Webbook
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
rinpol	2286.00		NIST Webbook
rinpol	2304.60		NIST Webbook
tb	647.40	K	Cheméo Relay (1.0)
tf	388.08	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.50	J/mol×K	739.37	Joback Method
cpg	428.46	J/mol×K	1008.22	Joback Method
cpg	423.09	J/mol×K	963.41	Joback Method
cpg	417.08	J/mol×K	918.60	Joback Method
cpg	410.38	J/mol×K	873.79	Joback Method

cpg	402.91	J/mol×K	828.99	Joback Method
cpg	394.64	J/mol×K	784.18	Joback Method
dvisc	0.0002798	Pa×s	614.71	Joback Method
dvisc	0.0001570	Pa×s	739.37	Joback Method
dvisc	0.0001860	Pa×s	697.82	Joback Method
dvisc	0.0002252	Pa×s	656.26	Joback Method
dvisc	0.0006694	Pa×s	490.04	Joback Method
dvisc	0.0003588	Pa×s	573.15	Joback Method
dvisc	0.0004783	Pa×s	531.60	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74472370&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):

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.