

2,2',4,5',6-Pentachlorobiphenyl

Other names:	2,2',4,5',6-Pentachlorobiphenyl PCB 103
Inchi:	InChI=1S/C12H5Cl5/c13-6-1-2-9(15)8(3-6)12-10(16)4-7(14)5-11(12)17/h1-5H
InchiKey:	PQHZWWBJPCNNGI-UHFFFAOYSA-N
Formula:	C12H5Cl5
SMILES:	Clc1cc(Cl)c(-c2cc(Cl)ccc2Cl)c(Cl)c1
Mol. weight [g/mol]:	326.44

Physical Properties

Property code	Value	Unit	Source
hf	78.42	kJ/mol	Cheméo Relay (1.0)
hfus	33.96	kJ/mol	Joback Method
hvap	91.60 ± 0.50	kJ/mol	NIST Webbook
ie	8.54	eV	Cheméo Relay (1.0)
log10ws	-7.44		Cheméo Relay (1.0)
logp	6.621		Crippen Method
mcvol	193.620	ml/mol	McGowan Method
tb	606.45	K	Cheméo Relay (1.0)
tf	356.52	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	394.64	J/mol×K	784.18	Joback Method
cpg	402.91	J/mol×K	828.99	Joback Method
cpg	410.38	J/mol×K	873.79	Joback Method
cpg	417.08	J/mol×K	918.60	Joback Method
cpg	423.09	J/mol×K	963.41	Joback Method
cpg	428.46	J/mol×K	1008.22	Joback Method
dvisc	0.0006694	Pa×s	490.04	Joback Method
dvisc	0.0004783	Pa×s	531.60	Joback Method
dvisc	0.0003588	Pa×s	573.15	Joback Method
dvisc	0.0002798	Pa×s	614.71	Joback Method

dvisc	0.0002252	Pa×s	656.26	Joback Method
dvisc	0.0001860	Pa×s	697.82	Joback Method
dvisc	0.0001570	Pa×s	739.37	Joback Method

Sources

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):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C60145213&Units=SI

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
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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