PCB 205

Other names:	PCB 205
	1,1'-Biphenyl, 2,3,3',4,4',5,5',6-octachloro
Inchi:	InChI=1S/C12H2Cl8/c13-4-1-3(2-5(14)7(4)15)6-8(16)10(18)12(20)11(19)9(6)17/h1-2H
InchiKey:	VXXBCDUYUQKWCK-UHFFFAOYSA-N
Formula:	C12H2Cl8
SMILES:	Clc1cc(-c2c(Cl)c(Cl)c(Cl)c(Cl)c2Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	429.77

Physical Properties

Property code	Value	Unit	Source
hf	38.93	kJ/mol	Cheméo Relay (1.0)
hfus	45.38	kJ/mol	Joback Method
hvap	114.62	kJ/mol	Cheméo Relay (1.0)
ie	8.69	eV	Cheméo Relay (1.0)
log10ws	-9.85		Cheméo Relay (1.0)
logp	8.581		Crippen Method
mcvol	230.340	ml/mol	McGowan Method
rinpol	2650.00		NIST Webbook
tb	668.72	K	Cheméo Relay (1.0)
tf	469.19	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	427.83	J/mol×K	866.60	Joback Method
cpg	433.76	J/mol×K	912.30	Joback Method
cpg	438.99	J/mol×K	958.00	Joback Method
cpg	443.56	J/mol×K	1003.70	Joback Method
cpg	447.49	J/mol×K	1049.40	Joback Method
cpg	450.83	J/mol×K	1095.11	Joback Method
cpg	453.59	J/mol×K	1140.81	Joback Method
dvisc	0.0003571	Pa×s	617.36	Joback Method
dvisc	0.0002775	Pa×s	658.90	Joback Method
dvisc	0.0002223	Pa×s	700.44	Joback Method

dvisc	0.0001825	Pa×s	741.98	Joback Method
dvisc	0.0001530	Pa×s	783.52	Joback Method
dvisc	0.0001305	Pa×s	825.06	Joback Method
dvisc	0.0001131	Pa×s	866.60	Joback Method

Sources

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C74472530&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):

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