Benzene, pentachloro-

Other names:	1,2,3,4,5-Pentachlorobenzene
	PCP
	Pentachlorobenzene
	QCB
	Rcra waste number U183
Inchi:	InChI=1S/C6HCl5/c7-2-1-3(8)5(10)6(11)4(2)9/h1H
InchiKey:	CEOCDNVZRAIOQZ-UHFFFAOYSA-N
Formula:	C6HCl5
SMILES:	Clc1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	250.34
CAS:	608-93-5

Physical Properties

Property code	Value	Unit	Source
chs	-2502.10 ± 0.80	kJ/mol	NIST Webbook
ea	0.73 ± 0.09	eV	NIST Webbook
gf	13.88	kJ/mol	Joback Method
hf	-40.00 ± 8.70	kJ/mol	NIST Webbook
hfus	24.77	kJ/mol	Joback Method
hsub	87.10 ± 0.40	kJ/mol	NIST Webbook
hvap	67.70	kJ/mol	NIST Webbook
ie	9.21 ± 0.03	eV	NIST Webbook
ie	8.80	eV	NIST Webbook
ie	9.11	eV	NIST Webbook
log10ws	-5.65		Estimated Solubility Method
log10ws	-5.65		Aqueous Solubility Prediction Method
logp	4.954		Crippen Method
mcvol	132.840	ml/mol	McGowan Method
pc	3427.87	kPa	Joback Method
rinpol	1510.54		NIST Webbook
rinpol	262.00		NIST Webbook
rinpol	260.10		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	260.09		NIST Webbook
rinpol	255.63		NIST Webbook

rinpol	1527.40		NIST Webbook
rinpol	1466.57		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1484.65		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1527.40		NIST Webbook
rinpol	1514.40		NIST Webbook
rinpol	1514.40		NIST Webbook
rinpol	1523.20		NIST Webbook
rinpol	1505.24		NIST Webbook
rinpol	1466.57		NIST Webbook
rinpol	262.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1505.00		NIST Webbook
rinpol	1525.00		NIST Webbook
rinpol	1487.83		NIST Webbook
rinpol	1502.28		NIST Webbook
rinpol	1501.00		NIST Webbook
rinpol	1504.00		NIST Webbook
rinpol	1492.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1483.00		NIST Webbook
rinpol	1509.00		NIST Webbook
rinpol	1478.00		NIST Webbook
rinpol	1496.00		NIST Webbook
rinpol	1546.00		NIST Webbook
rinpol	254.80		NIST Webbook
ripol	1998.10		NIST Webbook
ripol	2059.80		NIST Webbook
ripol	2028.86		NIST Webbook
ripol	2056.73		NIST Webbook
ripol	2037.50		NIST Webbook
ripol	2061.39		NIST Webbook
ripol	2027.00		NIST Webbook
ripol	1999.00		NIST Webbook
ripol	2026.20		NIST Webbook
tb	550.20	K	NIST Webbook
tc	821.83	K	Joback Method
tf	357.70 ± 0.20	K	NIST Webbook
tt	357.00 ± 0.03	K	NIST Webbook
vc	0.508	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	228.29	J/mol×K	821.83	Joback Method
cpg	202.34	J/mol×K	570.43	Joback Method
cpg	207.59	J/mol×K	612.33	Joback Method
cpg	212.45	J/mol×K	654.23	Joback Method
cpg	216.94	J/mol×K	696.13	Joback Method
cpg	221.06	J/mol×K	738.03	Joback Method
cpg	224.84	J/mol×K	779.93	Joback Method
dvisc	0.0002871	Pa×s	570.43	Joback Method
dvisc	0.0010893	Pa×s	383.48	Joback Method
dvisc	0.0008024	Pa×s	414.64	Joback Method
dvisc	0.0006168	Pa×s	445.80	Joback Method
dvisc	0.0004907	Pa×s	476.96	Joback Method
dvisc	0.0004015	Pa×s	508.11	Joback Method
dvisc	0.0003362	Pa×s	539.27	Joback Method
hfust	20.60	kJ/mol	357.70	NIST Webbook
hfust	20.10	kJ/mol	357.00	NIST Webbook
hfust	20.60	kJ/mol	357.70	NIST Webbook
hvapt	62.10	kJ/mol	460.00	NIST Webbook
hvapt	66.00	kJ/mol	357.00	NIST Webbook
sfust	56.30	J/mol×K	357.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.43191e+01
Coeff. B	-4.18161e+03
Coeff. C	-1.19138e+02
Temperature range (K), min.	417.16
Temperature range (K), max.	583.37

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C608935&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Determination of Henry's Law Constant Using Diffusion in Air and Water Boundary Layers:	https://www.doi.org/10.1021/je300954s
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
ea:	Electron affinity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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
pc:	Critical Pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume