pentachlorophenol

Other names: 2,3,4,5,6-Pentachlorophenol
Phenol, pentachloro-
penchlorol
Inchi: InChI=1S/C6HCl5O/c7-1-2(8)4(10)6(12)5(11)3(1)9/h12H
InchiKey: IZUPBVBPLAPZRR-UHFFFAOYSA-N
Formula: C6HCl5O
SMILES: Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 266.34
CAS: 87-86-5

Physical Properties

Property code	Value	Unit	Source
chs	-2329.70 ± 2.90	kJ/mol	NIST Webbook
gf	-140.74	kJ/mol	Joback Method
hf	-232.53	kJ/mol	Joback Method
hfs	-292.50 ± 3.00	kJ/mol	NIST Webbook
hfus	15.39	kJ/mol	Johari-Goldstein relaxation in orientationally disordered phase of hexa-substituted benzenes
hsub	91.60 ± 0.50	kJ/mol	NIST Webbook
hvap	68.81	kJ/mol	Joback Method
log10ws	-4.28		Estimated Solubility Method
log10ws	-4.44		Aqueous Solubility Prediction Method
logp	4.659		Crippen Method
mcvol	138.710	ml/mol	McGowan Method
pc	4114.41	kPa	Joback Method
rinpol	1743.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1748.00		NIST Webbook
rinpol	295.80		NIST Webbook
rinpol	296.78		NIST Webbook

rinpol	331.10		NIST Webbook
rinpol	1752.00		NIST Webbook
rinpol	1700.00		NIST Webbook
rinpol	1753.00		NIST Webbook
rinpol	1720.00		NIST Webbook
rinpol	1719.00		NIST Webbook
rinpol	1762.00		NIST Webbook
rinpol	1754.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1772.00		NIST Webbook
rinpol	1775.00		NIST Webbook
rinpol	1731.30		NIST Webbook
rinpol	1715.00		NIST Webbook
rinpol	1749.00		NIST Webbook
rinpol	1752.00		NIST Webbook
ripol	2821.00		NIST Webbook
ripol	2821.00		NIST Webbook
ripol	2848.00		NIST Webbook
ripol	2885.00		NIST Webbook
ripol	2855.00		NIST Webbook
ripol	2821.00		NIST Webbook
ss	253.17	J/mol×K	NIST Webbook
tb	583.20	K	NIST Webbook
tc	911.48	K	Joback Method
tf	462.50 ± 0.10	K	NIST Webbook
tf	463.84 ± 0.20	K	NIST Webbook
tf	462.80 ± 0.10	K	NIST Webbook
vc	0.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	231.90	J/mol×K	651.05	Joback Method
cpg	240.10	J/mol×K	737.86	Joback Method
cpg	243.82	J/mol×K	781.26	Joback Method
cpg	247.39	J/mol×K	824.67	Joback Method
cpg	250.89	J/mol×K	868.07	Joback Method
cpg	254.41	J/mol×K	911.48	Joback Method
cpg	236.15	J/mol×K	694.45	Joback Method
cps	201.96	J/mol×K	298.15	NIST Webbook

dvisc	0.0001643	Pa×s	521.17	Joback Method
dvisc	0.0001134	Pa×s	547.15	Joback Method
dvisc	0.0000809	Pa×s	573.12	Joback Method
dvisc	0.0000594	Pa×s	599.10	Joback Method
dvisc	0.0000448	Pa×s	625.07	Joback Method
dvisc	0.0002475	Pa×s	495.20	Joback Method
dvisc	0.0000346	Pa×s	651.05	Joback Method
hfust	17.15	kJ/mol	462.50	NIST Webbook
hvapt	69.00	kJ/mol	485.00	NIST Webbook
psub	9.75e-03	kPa	371.90	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.04	kPa	393.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.03	kPa	388.90	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.02	kPa	383.00	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

psub	0.02	kPa	378.10	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.06	kPa	397.80	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	6.81e-03	kPa	367.80	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	4.83e-03	kPa	363.00	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	3.04e-03	kPa	358.00	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	2.06e-03	kPa	353.10	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	1.27e-03	kPa	348.10	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.07	kPa	399.80	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
psub	0.09	kPa	403.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.88508e+01
Coeff. B	-8.30188e+03
Coeff. C	3.86753e-03
Coeff. D	-2.78260e-09
Temperature range (K), min.	463.15

Temperature range (K), max.	507.15

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
KDB:	https://www.cheric.org/files/research/kdb/mol/mol1792.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Johari-Goldstein relaxation in orientationally disordered phase of hexa-substituted benzenes?	https://www.doi.org/10.1016/j.tca.2015.01.017
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Liquid-liquid equilibrium (LLE) data for ternary mixtures of [C4DMIM][PF6] + [CP] + [water] and [C4DMIM][PF6] + [A] + [water] at T = 298.15 K and Thermochemistry of Chlorobenzenes and Chlorophenols: Ambiguous McGowan Method and Temperature Vapor Pressures and Enthalpies of Phase Transitions:	https://www.doi.org/10.1016/j.fluid.2014.08.004
NIST Webbook:	https://www.doi.org/10.1021/je060429r
KDB Vapor Pressure Data:	http://link.springer.com/article/10.1007/BF02311772
Joback Method:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C87865&Units=SI
Investigating the solubility of chlorophenols in hydrophobic ionic liquids:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1792
	https://en.wikipedia.org/wiki/Joback_method
	https://www.doi.org/10.1016/j.jct.2019.03.026

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
psub:	Sublimation pressure
pvap:	Vapor pressure
rinpol:	Non-polar retention indices

ripol:	Polar retention indices
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume