Phenol, 4-chloro-

Other names:	4-Chlorophenol
	4-Hydroxychlorobenzene
	Applied 3-78
	NSC 2877
	Parachlorophenol
	Phenol, p-chloro-
	p-Chlorfenol
	p-Chlorophenic acid
	p-Chlorophenol
Inchi:	InChI=1S/C6H5ClO/c7-5-1-3-6(8)4-2-5/h1-4,8H
InchiKey:	WXNZTHHGJRFXKQ-UHFFFAOYSA-N
Formula:	C6H5ClO
SMILES:	Oc1ccc(Cl)cc1
Mol. weight [g/mol]:	128.56
CAS:	106-48-9

Physical Properties

Property code	Value	Unit	Source
chl	-2917.90 ± 8.40	kJ/mol	NIST Webbook
chs	-2901.60 ± 8.40	kJ/mol	NIST Webbook
gf	-54.50	kJ/mol	Joback Method
hf	-123.69	kJ/mol	Joback Method
hfus	15.32	kJ/mol	Joback Method
hsub	77.10 ± 0.20	kJ/mol	NIST Webbook
hvap	64.40 ± 0.30	kJ/mol	NIST Webbook
ie	8.69	eV	NIST Webbook
ie	9.07	eV	NIST Webbook
log10ws	-0.70		Aqueous Solubility Prediction Method
log10ws	-0.70		Estimated Solubility Method
logp	2.046		Crippen Method
mcvol	89.750	ml/mol	McGowan Method
pc	5478.85	kPa	Joback Method
rinpol	1192.00		NIST Webbook
rinpol	1168.00		NIST Webbook
rinpol	1166.00		NIST Webbook

rinpol	1207.00		NIST Webbook
rinpol	1164.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1145.00		NIST Webbook
rinpol	1165.00		NIST Webbook
rinpol	1198.00		NIST Webbook
rinpol	1205.30		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1203.00		NIST Webbook
rinpol	1171.00		NIST Webbook
rinpol	1161.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1170.93		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1158.00		NIST Webbook
rinpol	1157.00		NIST Webbook
rinpol	1167.00		NIST Webbook
rinpol	1204.00		NIST Webbook
rinpol	1192.00		NIST Webbook
rinpol	1169.00		NIST Webbook
rinpol	1167.00		NIST Webbook
ripol	2335.00		NIST Webbook
ripol	2371.00		NIST Webbook
ripol	2371.00		NIST Webbook
ripol	2380.00		NIST Webbook
ripol	2364.00		NIST Webbook
ripol	2342.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2342.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2371.00		NIST Webbook
tb	492.90 ± 0.40	K	NIST Webbook
tb	492.90	K	NIST Webbook
tc	721.38	K	Joback Method
tf	316.10	K	Aqueous Solubility Prediction Method
tf	316.90	K	Crystalline and liquid vapour pressures of the four p-monohalophenols: A thermodynamic study of their phase transitions
tf	316.00 ± 0.20	K	NIST Webbook

tf	315.60	K	Solid liquid equilibria of mixtures containing tert-butanol, m-chlorophenol, and p-chlorophenol and development of adductive crystallization processes
tf	316.15	K	Liquid pharmaceuticals formulation by eutectic formation
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	167.36	J/mol×K	481.41	Joback Method
cpg	176.00	J/mol×K	521.40	Joback Method
cpg	183.82	J/mol×K	561.40	Joback Method
cpg	190.92	J/mol×K	601.39	Joback Method
cpg	197.38	J/mol×K	641.39	Joback Method
cpg	203.28	J/mol×K	681.38	Joback Method
cpg	208.73	J/mol×K	721.38	Joback Method
dvisc	0.0009700	Pa×s	377.43	Joback Method
dvisc	0.0019615	Pa×s	351.44	Joback Method
dvisc	0.0044385	Pa×s	325.44	Joback Method
dvisc	0.0005253	Pa×s	403.42	Joback Method
dvisc	0.0003064	Pa×s	429.42	Joback Method
dvisc	0.0001900	Pa×s	455.41	Joback Method
dvisc	0.0001241	Pa×s	481.41	Joback Method
hfust	14.07	kJ/mol	316.00	NIST Webbook
hfust	14.07	kJ/mol	315.90	NIST Webbook
hfust	14.07	kJ/mol	315.90	NIST Webbook
hsubt	54.00 ± 1.00	kJ/mol	297.00	NIST Webbook
hsubt	60.80	kJ/mol	272.50	NIST Webbook
hvapt	61.90	kJ/mol	334.50	NIST Webbook
hvapt	60.60	kJ/mol	433.00	NIST Webbook
hvapt	52.80	kJ/mol	408.00	NIST Webbook

psub	6.22e-03	kPa	297.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	2.36e-03	kPa	288.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	3.32e-03	kPa	291.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	4.59e-03	kPa	294.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	1.32e-03	kPa	283.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	8.39e-03	kPa	300.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.01	kPa	303.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.02	kPa	306.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.02	kPa	309.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
psub	0.03	kPa	311.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

psub	0.03	kPa	313.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
sfust	44.51	J/mol×K	316.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	2.47397e+01
Coeff. B	-8.31169e+03
Coeff. C	-2.54600e+01
Temperature range (K), min.	365.38
Temperature range (K), max.	453.28

Sources

Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C106489&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Solubilities of Some Chlorophenols in Supercritical CO2 in the Presence and Absence of Cosolvents:	https://www.doi.org/10.1021/je900328c
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Liquid pharmaceuticals formulation by eutectic formation:	https://www.doi.org/10.1016/j.fluid.2017.05.009
Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions:	https://www.doi.org/10.1021/je060429r
Crystalline and liquid vapour pressures of the four monochlorophenols: A thermodynamic study of their phase transitions:	https://www.doi.org/10.1016/j.jct.2013.05.047
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Solid liquid equilibria of mixtures containing tert-butanol, m-chlorophenol, and p-chlorophenol and development of adductive crystallization processes:	https://www.doi.org/10.1016/j.fluid.2005.08.021

Legend

chl:	Standard liquid enthalpy of combustion
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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
hsubt:	Enthalpy of sublimation at a given temperature
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
psub:	Sublimation 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
vc:	Critical Volume