Phenol, 2-chloro-

Other names:	1-Chloro-2-hydroxybenzene
	2-Chlorophenol
	2-Hydroxychlorobenzene
	NSC 2870
	Phenol, o-chloro-
	Rcra waste number U048
	o-Chlorophenic acid
	o-Chlorophenol
	o-Chlorphenol
Inchi:	InChI=1S/C6H5ClO/c7-5-3-1-2-4-6(5)8/h1-4,8H
InchiKey:	ISPYQTSUDJAMAB-UHFFFAOYSA-N
Formula:	C6H5ClO
SMILES:	Oc1ccccc1Cl
Mol. weight [g/mol]:	128.56
CAS:	95-57-8

Physical Properties

Property code	Value	Unit	Source
gf	-54.50	kJ/mol	Joback Method
hf	-123.69	kJ/mol	Joback Method
hfus	15.32	kJ/mol	Joback Method
hvap	52.30 ± 0.20	kJ/mol	NIST Webbook
ie	9.28	eV	NIST Webbook
log10ws	-1.06		Aqueous Solubility Prediction Method
log10ws	-1.06		Estimated Solubility Method
logp	2.046		Crippen Method
mcvol	89.750	ml/mol	McGowan Method
pc	5478.85	kPa	Joback Method
rinpol	990.00		NIST Webbook
rinpol	965.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	1002.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	987.00		NIST Webbook

rinpol	158.12		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	992.00		NIST Webbook
rinpol	952.00		NIST Webbook
rinpol	948.00		NIST Webbook
rinpol	947.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	1000.00		NIST Webbook
rinpol	993.00		NIST Webbook
rinpol	960.50		NIST Webbook
rinpol	967.30		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	973.00		NIST Webbook
rinpol	986.00		NIST Webbook
rinpol	987.00		NIST Webbook
rinpol	975.00		NIST Webbook
rinpol	979.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	156.80		NIST Webbook
ripol	1863.35		NIST Webbook
ripol	1866.00		NIST Webbook
ripol	1866.00		NIST Webbook
ripol	1812.00		NIST Webbook
ripol	1866.67		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1866.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1815.00		NIST Webbook
ripol	1788.00		NIST Webbook
ripol	1800.00		NIST Webbook
ripol	1830.00		NIST Webbook
ripol	1820.00		NIST Webbook
ripol	1868.14		NIST Webbook
ripol	1866.67		NIST Webbook
ripol	1861.01		NIST Webbook
tb	448.10	K	NIST Webbook
tb	448.90 ± 0.40	K	NIST Webbook
tb	450.00 ± 0.70	K	NIST Webbook
tb	448.15 ± 3.00	K	NIST Webbook
tc	721.38	K	Joback Method

tf	281.35	K	Aqueous Solubility Prediction Method
tf	281.15 ± 0.20	K	NIST Webbook
tf	282.00 ± 0.02	K	NIST Webbook
tf	281.15 ± 2.00	K	NIST Webbook
tf	283.00 ± 0.20	K	NIST Webbook
vc	0.279	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	176.00	J/mol×K	521.40	Joback Method
cpg	208.73	J/mol×K	721.38	Joback Method
cpg	203.28	J/mol×K	681.38	Joback Method
cpg	197.38	J/mol×K	641.39	Joback Method
cpg	190.92	J/mol×K	601.39	Joback Method
cpg	183.82	J/mol×K	561.40	Joback Method
cpg	167.36	J/mol×K	481.41	Joback Method
cpl	188.70	J/mol×K	283.00	NIST Webbook
dvisc	0.0009700	Pa×s	377.43	Joback Method
dvisc	0.0001241	Pa×s	481.41	Joback Method
dvisc	0.0001900	Pa×s	455.41	Joback Method
dvisc	0.0019615	Pa×s	351.44	Joback Method
dvisc	0.0005253	Pa×s	403.42	Joback Method
dvisc	0.0003064	Pa×s	429.42	Joback Method
dvisc	0.0044385	Pa×s	325.44	Joback Method
hfust	12.52	kJ/mol	283.00	NIST Webbook
hfust	12.52	kJ/mol	283.00	NIST Webbook
hfust	12.52	kJ/mol	283.00	NIST Webbook
hfust	0.09	kJ/mol	276.00	NIST Webbook
hvapt	51.90	kJ/mol	304.50	NIST Webbook
hvapt	47.00	kJ/mol	392.00	NIST Webbook
hvapt	47.20	kJ/mol	401.00	NIST Webbook
hvapt	50.10	kJ/mol	391.00	NIST Webbook
hvapt	45.20	kJ/mol	366.00	NIST Webbook

pvap	0.09	kPa	288.40	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
pvap	0.11	kPa	291.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
pvap	0.14	kPa	294.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
pvap	0.80	kPa	321.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
pvap	0.66	kPa	318.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions

pvap	0.56	kPa	315.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
pvap	0.46	kPa	312.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
pvap	0.38	kPa	309.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
pvap	0.31	kPa	306.20	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	
pvap	0.26	kPa	303.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions	

pvap	0.21	kPa	300.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
pvap	0.17	kPa	297.30	Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions
sfust	44.25	J/mol×K	283.00	NIST Webbook
sfust	0.33	J/mol×K	276.00	NIST Webbook
sfust	44.24	J/mol×K	283.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.72209e+01
Coeff. B	-5.60763e+03
Coeff. C	6.42200e+00
Temperature range (K), min.	324.74
Temperature range (K), max.	464.43

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Thermochemistry of Chlorobenzenes and Chlorophenols: Ambient Temperature Vapor Pressures and Enthalpies of Phase Transitions: https://www.doi.org/10.1021/je060429r

Joback Method: https://en.wikipedia.org/wiki/Joback_method

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=C95578&Units=SI
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
vc:	Critical Volume