p-Cresol

Other names:	1-Hydroxy-4-methylbenzene
	1-Methyl-4-hydroxybenzene
	4-Cresol
	4-Hydroxytoluene
	4-Methylphenol
	4-methylphenol (p-cresol)
	Cresol, para
	Cresol,p-
	NSC 3696
	Paracresol
	Paramethyl phenol
	Phenol, 4-methyl
	Phenol, 4-methyl-
	Rcra waste number U052
	p-Cresol (4-methylphenol)
	p-Cresylic acid
	p-Hydroxytoluene
	p-Kresol
	p-Methylhydroxybenzene
	p-Methylphenol
	p-Oxytoluene
	p-Toluol
	p-Tolyl alcohol
	para-cresol
	para-hydroxytoluene
Inchi:	InChI=1S/C7H8O/c1-6-2-4-7(8)5-3-6/h2-5,8H,1H3
InchiKey:	IWDCLRJOBJJRNH-UHFFFAOYSA-N
Formula:	C7H8O
SMILES:	Cc1ccc(O)cc1
Mol. weight [g/mol]:	108.14
CAS:	106-44-5

Physical Properties

Property code	Value	Unit	Source
affp	814.00 ± 8.00	kJ/mol	NIST Webbook
basg	782.00 ± 8.00	kJ/mol	NIST Webbook

chl	-3705.00	kJ/mol	NIST Webbook
chs	-3703.00	kJ/mol	NIST Webbook
chs	-3698.70 ± 0.30	kJ/mol	NIST Webbook
chs	-3698.60 ± 0.67	kJ/mol	NIST Webbook
gf	-34.15	kJ/mol	Joback Method
hf	-125.30 ± 1.50	kJ/mol	NIST Webbook
hf	-125.40 ± 1.50	kJ/mol	NIST Webbook
hfl	-193.00	kJ/mol	NIST Webbook
hfs	-199.20	kJ/mol	NIST Webbook
hfs	-199.30 ± 1.50	kJ/mol	NIST Webbook
hfus	13.71	kJ/mol	Joback Method
hsub	73.10 ± 0.60	kJ/mol	NIST Webbook
hsub	73.90	kJ/mol	NIST Webbook
hsub	73.90 ± 1.50	kJ/mol	NIST Webbook
hsub	73.90	kJ/mol	NIST Webbook
hvap	46.61	kJ/mol	NIST Webbook
ie	8.13	eV	NIST Webbook
ie	8.34	eV	NIST Webbook
ie	8.97	eV	NIST Webbook
ie	8.31 ± 0.08	eV	NIST Webbook
ie	8.38	eV	NIST Webbook
ie	8.34 ± 0.03	eV	NIST Webbook
ie	8.35	eV	NIST Webbook
log10ws	-0.73		Estimated Solubility Method
log10ws	-0.70		Aqueous Solubility Prediction Method
logp	1.701		Crippen Method
mcvol	91.600	ml/mol	McGowan Method
pc	5147.31 ± 81.06	kPa	NIST Webbook
pc	4559.63 ± 303.98	kPa	NIST Webbook
pc	4070.00 ± 58.84	kPa	NIST Webbook
rinpol	1086.00		NIST Webbook
rinpol	1085.74		NIST Webbook
rinpol	1089.67		NIST Webbook
rinpol	1076.00		NIST Webbook
rinpol	1078.00		NIST Webbook
rinpol	1080.00		NIST Webbook
rinpol	1081.00		NIST Webbook
rinpol	1082.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1056.00		NIST Webbook
rinpol	1054.00		NIST Webbook
rinpol	1064.00		NIST Webbook
rinpol	1066.00		NIST Webbook

rinpol	1048.00	NIST Webbook
rinpol	1074.00	NIST Webbook
rinpol	1075.00	NIST Webbook
rinpol	1078.00	NIST Webbook
rinpol	1093.00	NIST Webbook
rinpol	1080.00	NIST Webbook
rinpol	1077.30	NIST Webbook
rinpol	1076.00	NIST Webbook
rinpol	1075.30	NIST Webbook
rinpol	1093.00	NIST Webbook
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rinpol	1077.00	NIST Webbook
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rinpol	1044.00	NIST Webbook
rinpol	1104.00	NIST Webbook
rinpol	1048.00	NIST Webbook
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rinpol	175.80	NIST Webbook
rinpol	176.95	NIST Webbook
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rinpol	1059.00	NIST Webbook
rinpol	1093.00	NIST Webbook
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ripol	2083.00	NIST Webbook
ripol	2100.00	NIST Webbook
ripol	2094.21	NIST Webbook
ripol	2100.99	NIST Webbook
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ripol	2049.00	NIST Webbook
ripol	2100.00	NIST Webbook
ripol	2067.00	NIST Webbook
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ripol	2050.00		NIST Webbook
ripol	2089.00		NIST Webbook
ripol	2103.00		NIST Webbook
ripol	2047.00		NIST Webbook
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ripol	2078.00		NIST Webbook
ripol	2038.00		NIST Webbook
ripol	2037.00		NIST Webbook
ripol	2074.00		NIST Webbook
ripol	2090.00		NIST Webbook
ripol	2076.00		NIST Webbook
ripol	2087.00		NIST Webbook
ripol	2053.00		NIST Webbook
ripol	2073.00		NIST Webbook
ripol	2089.00		NIST Webbook
ss	167.32	J/mol×K	NIST Webbook
tb	474.85 ± 1.00	K	NIST Webbook
tb	473.70 ± 1.00	K	NIST Webbook
tb	475.65 ± 1.00	K	NIST Webbook
tb	475.65 ± 0.20	K	NIST Webbook
tb	475.47 ± 1.00	K	NIST Webbook

tb	474.85 ± 0.40	K	NIST Webbook
tb	475.25 ± 1.00	K	NIST Webbook
tb	475.15 ± 1.00	K	NIST Webbook
tb	475.03 ± 0.30	K	NIST Webbook
tb	474.65 ± 1.00	K	NIST Webbook
tb	475.05 ± 0.40	K	NIST Webbook
tb	475.10	K	NIST Webbook
tb	474.85	K	Experimental and predicted vapor-liquid equilibrium for binary systems with diethanolamine, m-cresol and p-cresol at 20.0 kPa
tb	474.95 ± 2.00	K	NIST Webbook
tc	704.55 ± 0.30	K	NIST Webbook
tc	704.60 ± 0.40	K	NIST Webbook
tc	699.20 ± 5.00	K	NIST Webbook
tc	699.00 ± 3.00	K	NIST Webbook
tf	306.05	K	Aqueous Solubility Prediction Method
tf	307.00 ± 0.10	K	NIST Webbook
tf	309.00 ± 1.00	K	NIST Webbook
tf	307.15 ± 0.50	K	NIST Webbook
tf	306.95 ± 0.20	K	NIST Webbook
tf	305.15 ± 0.50	K	NIST Webbook
tf	307.30 ± 0.30	K	NIST Webbook
tf	307.70 ± 0.20	K	NIST Webbook
tf	307.55 ± 0.60	K	NIST Webbook
tf	306.15 ± 1.50	K	NIST Webbook
tf	307.55 ± 0.50	K	NIST Webbook
tf	307.75 ± 0.30	K	NIST Webbook
tf	307.85 ± 0.50	K	NIST Webbook
tf	307.93 ± 0.10	K	NIST Webbook
tf	307.88 ± 0.05	K	NIST Webbook
tf	307.15 ± 1.00	K	NIST Webbook
tf	307.84 ± 0.05	K	NIST Webbook
tt	307.94 ± 0.02	K	NIST Webbook
vc	0.285	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	237.56	J/mol×K	696.68	Joback Method

cpg	184.27	J/mol×K	466.86	Joback Method
cpg	204.98	J/mol×K	543.47	Joback Method
cpg	214.11	J/mol×K	581.77	Joback Method
cpg	222.53	J/mol×K	620.08	Joback Method
cpg	230.32	J/mol×K	658.38	Joback Method
cpg	195.06	J/mol×K	505.16	Joback Method
cps	226.20	J/mol×K	313.00	NIST Webbook
cps	163.50	J/mol×K	298.15	NIST Webbook
cps	221.03	J/mol×K	298.15	NIST Webbook
cps	150.25	J/mol×K	298.15	NIST Webbook
dvisc	0.0032450	Pa×s	333.15	Excess Molar Volumes and Viscosities of Binary Mixtures of p-Cresol with Ethylene Glycol and Methanol at Different Temperature and Atmospheric Pressure
dvisc	0.0018910	Pa×s	353.15	Excess Molar Volumes and Viscosities of Binary Mixtures of p-Cresol with Ethylene Glycol and Methanol at Different Temperature and Atmospheric Pressure
dvisc	0.0067450	Pa×s	313.15	Excess Molar Volumes and Viscosities of Binary Mixtures of p-Cresol with Ethylene Glycol and Methanol at Different Temperature and Atmospheric Pressure
dvisc	0.0038880	Pa×s	328.15	Excess Molar Volumes and Viscosities of Binary Mixtures of p-Cresol with Ethylene Glycol and Methanol at Different Temperature and Atmospheric Pressure

dvisc	0.0045320	Pa×s	323.15	Excess Molar Volumes and Viscosities of Binary Mixtures of p-Cresol with Ethylene Glycol and Methanol at Different Temperature and Atmospheric Pressure
dvisc	0.0054710	Pa×s	318.15	Excess Molar Volumes and Viscosities of Binary Mixtures of p-Cresol with Ethylene Glycol and Methanol at Different Temperature and Atmospheric Pressure
dvisc	0.0084440	Pa×s	308.15	Excess Molar Volumes and Viscosities of Binary Mixtures of p-Cresol with Ethylene Glycol and Methanol at Different Temperature and Atmospheric Pressure
dvisc	0.0024310	Pa×s	343.15	Excess Molar Volumes and Viscosities of Binary Mixtures of p-Cresol with Ethylene Glycol and Methanol at Different Temperature and Atmospheric Pressure
hfust	11.89	kJ/mol	309.00	NIST Webbook
hfust	12.71	kJ/mol	307.94	NIST Webbook
hfust	12.60	kJ/mol	308.80	NIST Webbook
hfust	12.72	kJ/mol	307.90	NIST Webbook
hfust	8.58	kJ/mol	307.60	NIST Webbook
hfust	12.25	kJ/mol	309.00	NIST Webbook
hfust	11.80	kJ/mol	307.40	NIST Webbook
hfust	12.72	kJ/mol	307.90	NIST Webbook
hfust	11.80	kJ/mol	307.35	NIST Webbook
hsubt	73.90 ± 1.50	kJ/mol	290.00	NIST Webbook
hvapt	55.40	kJ/mol	431.00	NIST Webbook
hvapt	49.20	kJ/mol	498.00	NIST Webbook
hvapt	55.60	kJ/mol	428.00	NIST Webbook
hvapt	51.30	kJ/mol	446.50	NIST Webbook

hvapt	46.00	kJ/mol	579.00	NIST Webbook
hvapt	62.00	kJ/mol	350.50	NIST Webbook
rfi	1.53100		308.15	Densities, Speeds of Sound, and Refractive Indices of Binary Mixtures of Decan-1-ol with Anisole, o-Cresol, m-Cresol, and p-Cresol at T = (298.15, 303.15, and 308.15) K
rfi	1.53900		298.15	Activity coefficients of the binary mixtures of a-cresol or p-cresol with C l-C4 aliphatic alcohols near ambient pressure
rfi	1.53910		298.15	Excess Gibbs' energies of the binary mixtures formed by N,N-dimethylformamide with xylenes and cresols at 95.1 kPa
rfi	1.53910		298.15	Activity coefficients and excess Gibbs free energy of some binary mixtures formed by p-cresol at 95.23 kPa
rfi	1.53700		298.15	Densities, Speeds of Sound, and Refractive Indices of Binary Mixtures of Decan-1-ol with Anisole, o-Cresol, m-Cresol, and p-Cresol at T = (298.15, 303.15, and 308.15) K

rfi	1.53400		303.15	Densities, Speeds of Sound, and Refractive Indices of Binary Mixtures of Decan-1-ol with Anisole, o-Cresol, m-Cresol, and p-Cresol at T = (298.15, 303.15, and 308.15) K
rfi	1.53910		298.15	Excess Gibbs energies of binary mixtures formed by nitrobenzene with selected compounds at 94.95 kPa
rhol	1006.72	kg/m3	328.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1026.39	kg/m3	303.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1030.25	kg/m3	298.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1034.09	kg/m3	293.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1025.90	kg/m3	303.15	Vapor-Liquid Equilibria in Ternary Systems of Toluene or Octane + Phenols + Water

rhol	1018.80	kg/m3	313.15	Liquid-Liquid(-Liquid) Equilibria in Ternary Systems of Aliphatic Hydrocarbons (Heptane or Octane) + Phenols + Water
rhol	1014.68	kg/m3	318.15	Thermodynamic and spectroscopic study of molecular interactions between ethanol and isomeric cresols
rhol	1022.50	kg/m3	308.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1014.66	kg/m3	318.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1022.56	kg/m3	308.15	Thermodynamic and spectroscopic study of molecular interactions between ethanol and isomeric cresols
rhol	1026.47	kg/m3	303.15	Thermodynamic and spectroscopic study of molecular interactions between ethanol and isomeric cresols
rhol	1011.30	kg/m3	323.20	Liquid-liquid equilibrium for methyl butyl ketone + o-, m-, p-cresol + water ternary systems and COSMO-SAC predictions

rhol	1154.00	kg/m3	298.15	Bubble point measurements of binary mixtures formed by ethyl benzene with selected compounds at 95.35 kPa
rhol	1018.59	kg/m3	313.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1010.70	kg/m3	323.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	994.59	kg/m3	343.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	998.66	kg/m3	338.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1002.70	kg/m3	333.15	Experimental Densities and Speeds of Sound of Substituted Phenols and Their Modeling with the Prigogine Flory Patterson Model
rhol	1018.64	kg/m3	313.15	Thermodynamic and spectroscopic study of molecular interactions between ethanol and isomeric cresols

rhol	1018.80	kg/m3	313.15	Liquid-Liquid Equilibria in Ternary Systems of Aromatic Hydrocarbons (Toluene or Ethylbenzene) + Phenols + Water
sfust	38.47	J/mol×K	309.00	NIST Webbook
sfust	41.26	J/mol×K	307.94	NIST Webbook
sfust	39.60	J/mol×K	309.00	NIST Webbook
sfust	38.00	J/mol×K	307.35	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.76963e+02
Coeff. B	-1.46480e+04
Coeff. C	-2.33776e+01
Coeff. D	1.14084e-05
Temperature range (K), min.	307.93
Temperature range (K), max.	704.65

Datasets

Mass density, kg/m3

Temperature, K - Liquid	Pressure, kPa - Liquid	Mass density, kg/m3 - Liquid
312.90	1002.00	1019.4
312.90	2016.00	1020.0
312.90	3017.00	1020.6
312.90	4016.00	1021.1
312.90	5002.00	1021.7
312.90	6010.00	1022.2
312.90	7000.00	1022.8
312.90	8006.00	1023.3

312.90	9001.00	1023.9
312.90	10002.00	1024.4
312.90	11006.00	1024.9
312.90	12002.00	1025.5
312.90	13015.00	1026.0
312.90	14007.00	1026.6
312.90	15006.00	1027.1
312.90	16019.00	1027.6
312.90	17004.00	1028.1
312.90	18011.00	1028.6
312.90	19009.00	1029.2
312.90	20005.00	1029.7
312.90	21008.00	1030.2
312.90	22004.00	1030.7
312.90	23023.00	1031.2
312.90	24004.00	1031.7
312.90	25006.00	1032.2
322.78	1019.00	1011.6
322.78	2015.00	1012.2
322.78	3002.00	1012.8
322.78	4013.00	1013.4
322.78	5011.00	1013.9
322.78	6018.00	1014.5
322.78	7022.00	1015.1
322.78	8001.00	1015.7
322.78	9015.00	1016.3
322.78	10006.00	1016.8
322.78	11002.00	1017.4
322.78	12018.00	1017.9
322.78	13002.00	1018.4
322.78	14016.00	1019.0
322.78	15001.00	1019.5
322.78	16000.00	1020.1
322.78	17001.00	1020.6
322.78	18029.00	1021.2
322.78	19015.00	1021.7
322.78	20011.00	1022.2
322.78	21022.00	1022.8
322.78	22002.00	1023.3
322.78	23006.00	1023.8
322.78	24010.00	1024.4
322.78	25023.00	1024.9
332.54	1040.00	1003.7
332.54	2019.00	1004.3

332.54	3013.00	1005.0
332.54	4019.00	1005.6
332.54	5001.00	1006.2
332.54	6001.00	1006.8
332.54	7002.00	1007.5
332.54	8041.00	1008.1
332.54	9000.00	1008.7
332.54	10001.00	1009.2
332.54	11006.00	1009.7
332.54	12001.00	1010.4
332.54	13008.00	1010.9
332.54	14004.00	1011.5
332.54	15003.00	1012.1
332.54	16015.00	1012.7
332.54	17011.00	1013.3
332.54	18014.00	1013.9
332.54	19014.00	1014.4
332.54	20009.00	1014.9
332.54	21013.00	1015.4
332.54	22007.00	1016.0
332.54	23000.00	1016.6
332.54	24001.00	1017.1
332.54	25032.00	1017.7
342.37	1001.00	995.7
342.37	2002.00	996.4
342.37	3004.00	997.1
342.37	4025.00	997.7
342.37	5036.00	998.2
342.37	6032.00	998.8
342.37	7001.00	999.3
342.37	8020.00	999.9
342.37	9003.00	1000.6
342.37	10002.00	1001.3
342.37	11036.00	1001.9
342.37	12001.00	1002.6
342.37	13020.00	1003.2
342.37	14019.00	1003.9
342.37	15007.00	1004.5
342.37	16000.00	1005.1
342.37	17022.00	1005.6
342.37	18014.00	1006.2
342.37	19033.00	1006.8
342.37	20005.00	1007.4
342.37	21005.00	1007.9

342.37	22010.00	1008.4
342.37	22962.00	1009.0
342.37	24021.00	1009.7
342.37	25017.00	1010.2
352.15	1023.00	987.9
352.15	2007.00	988.5
352.15	3000.00	989.1
352.15	4003.00	989.8
352.15	5001.00	990.4
352.15	6009.00	991.1
352.15	7001.00	991.7
352.15	8037.00	992.4
352.15	9008.00	993.0
352.15	10040.00	993.7
352.15	11006.00	994.3
352.15	12001.00	994.9
352.15	13001.00	995.5
352.15	14009.00	996.2
352.15	15000.00	996.8
352.15	16010.00	997.4
352.15	17028.00	998.0
352.15	18020.00	998.6
352.15	19045.00	999.3
352.15	20018.00	1000.0
352.15	21038.00	1000.5
352.15	22000.00	1001.1
352.15	23065.00	1001.8
352.15	24024.00	1002.4
352.15	25039.00	1002.9
361.90	1017.00	979.6
361.90	1991.00	980.3
361.90	3004.00	981.0
361.90	4027.00	981.5
361.90	4992.00	982.3
361.90	6000.00	983.1
361.90	7033.00	983.6
361.90	8010.00	984.4
361.90	9001.00	985.0
361.90	9998.00	985.8
361.90	10994.00	986.5
361.90	11976.00	987.0
361.90	12949.00	987.7
361.90	14010.00	988.3
361.90	15017.00	989.0

361.90	15992.00	989.6
361.90	16992.00	990.3
361.90	18007.00	990.8
361.90	19034.00	991.6
361.90	19992.00	992.1
361.90	21000.00	992.9
361.90	22059.00	993.4
361.90	23020.00	994.1
361.90	24014.00	994.8
361.90	25002.00	995.3

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	https://www.doi.org/10.1021/je100362p

Legend

affp:	Proton affinity
basg:	Gas basicity
chl:	Standard liquid enthalpy of combustion
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
hfl:	Liquid phase 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
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
pvap:	Vapor pressure
rfi:	Refractive Index
rhol:	Liquid Density

rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tt:	Triple Point Temperature
vc:	Critical Volume