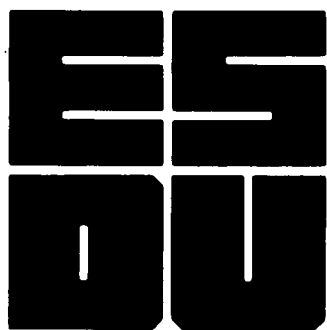


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Engineering Sciences Data

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Vapour pressures and critical points of liquids

XX: Additional derivatives of phenol

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The work on this Item was carried out in the Internal Flow and Physical Properties Group of the Engineering Sciences Data Unit under the supervision of Mr R.Partington, Group Head. The member of staff who undertook the construction and subsequent development of the Item was

Mr J.Walton — Senior Engineer.

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* Corresponding Member

VAPOUR PRESSURES AND CRITICAL POINTS OF LIQUIDS XX: ADDITIONAL DERIVATIVES OF PHENOL

1. INTRODUCTION

This Data Item presents saturated vapour pressures of the additional derivatives of phenol listed in Table I (pages 2 and 3).

The range and quality of the experimental data for each compound, on which the tabulated values are based is discussed in Section A.1 of Appendix A.

Table I shows, for each compound, alternative names, empirical and structural formulae, molecular weight, normal boiling point, dT/dp at the normal boiling point and acentric factor. The name in bold type is that based on BSI Recommendations.

Tables II to V present values of vapour pressure, in kPa, at 5 K intervals of temperature down to a temperature either just above the melting point, or at which the pressure is approximately 0.001 kPa, whichever is the higher. For those compounds which are known or considered likely to be thermally stable up to the critical point, the Tables extend over the whole temperature range. However some of the compounds considered here are known, or thought, to decompose at temperatures well below their estimated critical value, so for these compounds the estimated values of critical temperature and pressure, T_c and p_c , used in the vapour pressure equation are given, but the vapour pressures in Tables II to V terminate at a lower convenient arbitrary temperature.

The values of vapour pressure given in the Tables were obtained by evaluating, for each compound, a Wagner equation of the form

$$\log_e p = \log_e p_c + (T_c/T)[b_1 q + b_2 q^{3/2} + b_3 q^3 + b_4 q^6] \quad (1)$$

where $q = 1 - T/T_c$.

This equation had been fitted to the experimental data that had been selected and weighted in accordance with a critical assessment of all the data. Table VI gives T , $\log_e p$ and the coefficients b_1, b_2, b_3, b_4 for each compound that, when used in Equation (1), give p in kPa for T in kelvins.

The suggested uncertainties in the tabulated values of vapour pressure that the user should allow for are discussed and tabulated in Appendix A.

The location of the Table giving the vapour pressure values for each compound is shown on the foldout flap attached to the last page.

A full explanation of the correlation procedure used to derive the tabulated values of vapour pressure together with notation and units, a simple interpolation procedure, conversion factors and References is given in the introductory Data Item, Reference 1.

2. REFERENCES

1. ESDU Vapour pressures and critical points of liquids. Introduction to Data Items issued after July 1980. Item No. 80016, Engineering Sciences Data Unit, 1980.

TABLE I (Part 1)
Additional Derivatives of Phenol

No.	Name	Alternative Names	
(Name based on BSI Recommendations in Bold Type)			
1	C ₆ H ₅ ClO	2-Chlorophenol	
2	C ₆ H ₅ ClO	3-Chlorophenol	
3	C ₆ H ₅ ClO	4-Chlorophenol	
4	C ₆ H ₄ Cl ₂ O	2,4-Dichlorophenol	
5	C ₆ H ₄ Cl ₂ O	2,6-Dichlorophenol	
6	C ₆ H ₃ Cl ₃ O	2,4,5-Trichlorophenol	
7	C ₆ H ₃ Cl ₃ O	2,4,6-Trichlorophenol	
8	C ₆ H ₃ BrCl ₂ O	2-Bromo-4,6-dichlorophenol	
9	C ₆ H ₂ Cl ₄ O	2,3,4,6-Tetrachlorophenol	
10	C ₆ H ₂ BrCl ₃ O	3-Bromo-2,4,6-trichlorophenol	
11	C ₆ HF ₅ O	Pentafluorophenol	
12	C ₆ HCl ₅ O	Pentachlorophenol	
13	C ₆ H ₅ NO ₃	2-Nitrophenol	
14	C ₆ H ₅ NO ₃	3-Nitrophenol	
15	C ₆ H ₅ NO ₃	4-Nitrophenol	
16	C ₆ H ₆ O ₂	1,2-Dihydroxybenzene	Catechol
17	C ₆ H ₆ O ₂	1,3-Dihydroxybenzene	Resorcinol
18	C ₆ H ₆ O ₂	1,4-Dihydroxybenzene	Quinol
			Pyrocatechol
			Hydroquinone
19	C ₆ H ₆ O ₃	1,2,3-Trihydroxybenzene	Pyrogallol
20	C ₇ H ₈ O ₂	2-Methoxyphenol	Guaiacol
21	C ₁₂ H ₁₀ O	2-Phenylphenol	2-Hydroxybiphenyl
22	C ₁₂ H ₁₀ O	4-Phenylphenol	4-Hydroxybiphenyl
23	C ₁₂ H ₁₀ O ₂	2,2'-Biphenol	2,2'-Dihydroxybiphenyl
24	C ₁₄ H ₁₄ O	2-Phenylethylphenol	
25	C ₁₄ H ₁₄ O	4-Phenylethylphenol	
26	C ₁₀ H ₈ O	1-Naphthol	1-Hydroxynaphthalene
27	C ₁₀ H ₈ O	2-Naphthol	2-Hydroxynaphthalene
28	C ₉ H ₁₀ O	Indan-5-ol	5-Hydroxyindane
29	C ₁₂ H ₈ O	Dibenzofuran	Diphenylene oxide

TABLE I (Part 2)
General Information

No.	Name	M.W.	Structural Formula	Normal Boiling Point				Acentric Factor ω
				$p = 101.325 \text{ kPa}$		$p = 760 \text{ mmHg}$		
				T K	dT/dp K/kPa	t °C	dt/dp °C/mmHg	
1	2-Chlorophenol	128.558	2-ClC ₆ H ₄ OH	447.53	0.3923	174.38	0.05230	0.435
2	3-Chlorophenol	128.558	3-ClC ₆ H ₄ OH	487.00	0.4046	213.85	0.05394	0.497
3	4-Chlorophenol	128.558	4-ClC ₆ H ₄ OH	493.11	0.4067	219.96	0.05422	0.490
4	2,4-Dichlorophenol	163.003	2,4-Cl ₂ C ₆ H ₃ OH	483.02	0.3796	209.87	0.05061	0.459
5	2,6-Dichlorophenol	163.003	2,6-Cl ₂ C ₆ H ₃ OH	493.57	0.3875	220.42	0.05166	0.463
6	2,4,5-Trichlorophenol	197.448	2,4,5-Cl ₃ C ₆ H ₂ OH	525.72	0.4359	252.57	0.05812	0.458
7	2,4,6-Trichlorophenol	197.448	2,4,6-Cl ₃ C ₆ H ₂ OH	520.47	0.4160	247.32	0.05546	0.468
8	2-Bromo-4,6-dichlorophenol	241.899	2-Br-4,6-Cl ₂ C ₆ H ₂ OH	542.94	0.4494	269.79	0.05992	0.450
9	2,3,4,6-Tetrachlorophenol	231.893	2,3,4,6-Cl ₄ C ₆ HOH	549.73	0.4346	276.58	0.05794	0.475
10	3-Bromo-2,4,6-trichlorophenol	276.344	3-Br-2,4,6-Cl ₃ C ₆ HOH	580.15	0.4679	307.00	0.06238	0.461
11	Pentafluorophenol	184.065	C ₆ F ₅ OH	418.79	0.3376	145.64	0.04501	0.503
12	Pentachlorophenol	266.338	C ₆ Cl ₅ OH	584.50	0.4405	311.35	0.05872	0.505
13	2-Nitrophenol	139.110	2-NO ₂ C ₆ H ₄ OH	488.29	0.3816	215.14	0.05087	0.597
14	3-Nitrophenol	139.110	3-NO ₂ C ₆ H ₄ OH	545.33	0.3971	272.18	0.05294	0.664
15	4-Nitrophenol	139.110	4-NO ₂ C ₆ H ₄ OH	552.00	0.4024	278.85	0.05365	0.660
16	1,2-Dihydroxybenzene	110.112	1,2-(OH) ₂ C ₆ H ₄	517.54	0.3946	244.39	0.05261	0.585
17	1,3-Dihydroxybenzene	110.112	1,3-(OH) ₂ C ₆ H ₄	549.29	0.3867	276.14	0.05156	0.636
18	1,4-Dihydroxybenzene	110.112	1,4-(OH) ₂ C ₆ H ₄	558.47	0.3905	285.32	0.05206	0.659
19	1,2,3-Trihydroxybenzene	126.112	1,2,3-(OH) ₃ C ₆ H ₃	581.59	0.4038	308.44	0.05384	0.723
20	2-Methoxyphenol	124.139	2-CH ₃ OC ₆ H ₄ OH	477.11	0.3942	203.96	0.05256	0.476
21	2-Phenylphenol	170.210	2-C ₆ H ₅ C ₆ H ₄ OH	550.79	0.4184	277.64	0.05578	0.546
22	4-Phenylphenol	170.210	4-C ₆ H ₅ C ₆ H ₄ OH	583.34	0.4353	310.19	0.05803	0.592
23	2,2'-Biphenol	186.210	[2-(OH)C ₆ H ₄] ₂	597.28	0.4653	324.13	0.06204	0.682
24	2-Phenylethylphenol	198.264	2-(C ₆ H ₅ C ₂ H ₄)C ₆ H ₄ OH	593.01	0.4707	319.86	0.06276	0.617
25	4-Phenylethylphenol	198.264	4-(C ₆ H ₅ C ₂ H ₄)C ₆ H ₄ OH	603.01	0.4632	329.86	0.06175	0.614
26	1-Naphthol	144.173	1-(OH)C ₁₀ H ₇	555.24	0.4454	282.09	0.05936	0.476
27	2-Naphthol	144.173	2-(OH)C ₁₀ H ₇	560.13	0.4514	286.98	0.06018	0.488
28	Indan-5-ol	134.137	5-(OH)C ₉ H ₉	526.09	0.4192	252.94	0.05589	0.486
29	Dibenzofuran	168.195	C ₁₂ H ₈ O	559.29	0.5234	286.14	0.06978	0.315