

NOTE

New values of the polarity factor

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New values of the polarity factor χ for 96 substances are proposed. Estimation procedure is tested on the values of this factor from the original work of Halm and Stiel.⁴⁴

Keywords: polarity factor, acentric factor, vapor pressure.

Halm and Stiel⁴⁴ have proposed following relation for predicting vapor pressure of a polar fluid

$$\log p_r^0 = (\log p_r^0)^{(0)} + \omega(\log p_r^0)^{(1)} + \chi (\log p_r^0)^{(2)} \quad (1)$$

where χ is polarity factor similar to the acentric factor for normal fluids. The factor χ is defined to be zero for normal fluids. The values of $(\log p_r^0)^{(0)}$, $(\log p_r^0)^{(1)}$, and $(\log p_r^0)^{(2)}$ vs. temperature are tabulated in original work. The value of $(\log p_r^0)^{(2)}$ was defined to be 1.0 at $T_r = 0.6$, so that

$$\chi = \log p_r^0|_{T_r=0.6} - [(\log p_r^0)^{(0)} + \omega(\log p_r^0)^{(1)}]_{T_r=0.6} \quad (2)$$

or

$$\chi = \log p_r^0|_{T_r=0.6} + 1.552 + 1.7 \omega \quad (3)$$

RESULTS AND DISCUSSION

Polarity factor estimated values are shown Table I. The values of T_c , p_c and ω used in this estimation and sources of the experimental vapor pressure data used to establish the values of χ are also included in this Table.

TABLE I. The values of the polarity factor

Substance	χ	Substance	χ	Substance	χ
1. Acetaldehyde	0.034	33. 2,4-Dimethylphenol	0.021	65. 3-Methyl-2-butanone	0.007
2. Acetone	0.007	34. 2,5-Dimethylphenol	-0.024	66. Methylbutylether	0.008
3. Acetonitrile	0.048	35. 3,5-Dimethylphenol	0.016	67. Methylbutyrate	-0.001
4. Ammonia	0.003	36. 2,3-Dimethylpyridine	-0.039	68. Methylformate	-0.009
5. Aniline	0.007	37. 2,4-Dimethylpyridine	-0.006	69. <i>o</i> -Methylphenol	-0.004
6. Benzaldehyde	0.017	38. 2,6-Dimethylpyridine	-0.003	70. <i>p</i> -Methylphenol	0.009
7. Bromobenzene	0.002	39. 3,5-Dimethylpyridine	-0.015	71. Methylphenylether	0.081
8. Bromoethane	0.035	40. Dimethylsulfide	0.003	72. Methylpropanoate	0.012
9. Bromomethane	0.039	41. Dipropylether	0.019	73. 2-Methyl-1-propanol	-0.069
10. 2-Butanone	0.036	42. 1-Dodecanol	0.044	74. 2-Methyl-2-propanol	-0.097
11. Butylacetate	-0.004	43. Dichloromethane	-0.014	75. Methylpropylether	0.006
12. Butylamine	-0.004	44. Ethanol	0.002	76. 2-Methylpyridine	0.005
13. Butyric acide	-0.009	45. Ethanolamine	0.048	77. 3-Methylpyridine	0.004
14. Butyronitrile	0.027	46. Ethylbutylether	0.030	78. Morpholine	0.022
15. Capronitrile	0.063	47. Ethylformate	-0.009	79. Nitromethane	0.038
16. Chlorobenzene	-0.018	48. Ethylenediamine	0.089	80. 5-Nonanone	0.019
17. 1-Chlorobutane	-0.026	49. Ethyleneoxide	0.012	81. 1-Octanol	-0.083
18. Chloroethane	0.006	50. Ethylpropionate	-0.002	82. 1-Pentanol	-0.046
19. Chloroethene	-0.019	51. Ethylpropylether	0.016	83. 3-Pentanone	-0.010
20. Chloromethane	0.020	52. Ethylacetate	0.038	84. Phenol	-0.001
21. Cyclohexanone	0.071	53. Fluorobenzene	-0.001	85. 2-Propanol	-0.054
22. Dibutylether	-0.025	54. Fluoroethane	0.008	86. Propionic acid	-0.039
23. <i>m</i> -Dichlorobenzene	0.024	55. Formaldehyde	-0.015	87. Propionitrile	0.006
24. <i>o</i> -Dichlorobenzene	-0.006	56. Hydrogenchloride	0.025	88. Propylacetate	-0.004
25. 1,2-Dichloropropane	-0.005	57. Hydrogenfluoride	0.037	89. Pyridine	-0.020
26. Diethylamine	-0.014	58. Iodoethane	0.062	90. Sulfur dioxide	0.004
27. Diethylether	-0.011	59. Isobutylamine	0.053	91. 1,1,2,2-Tetrachloroethane	-0.028
28. Diethylsulfide	-0.001	60. Methanoic acid	0.024	92. Thiacyclopentane	0.019
29. Diethylsulfide	0.008	61. Methanol	0.040	93. 1,1,1-Trichloroethane	0.001
30. Diisopropylamine	0.026	62. Methylacetate	0.004	94. Trichloromethane	0.013
31. Dimethylamine	-0.001	63. Methylbenzoate	0.020	95. 1,1,1-Trifluoroethane	0.001
32. Dimethylether	0.016	64. 2-Methyl-2-butanol	-0.090	96. Water	0.023

1. Acetaldehyde (vapor pressure references $24/T_c(K) = 461.0/p_c(\text{bar}) = 55.7/\omega = 0.303$), **2.** (9, 30, 33, 55, 62, 73, 85/508.1/47.0/0.307), **3.** (30, 67/545.5/48.3/0.327), **4.** (14, 19, 74, 95, 109/405.5/113.5/0.215), **5.** (30, 51, 81/699.0/53.1/0.384), **6.** (1, 27, 41, 51, 82/694.8/45.4/0.316), **7.** (30, 51, 81, 108/670.0/45.2/0.250), **8.** (56/503.9/62.3/0.229), **9.** (31, 56/464.0/66.1/0.157), **10.** (30, 55/536.8/42.1/0.318), **11.** (54/579.0/31.4/0.417), **12.** (41, 59/531.9/42.0/0.329), **13.** (49, 50/628.0/52.7/0.683), **14.** (66, 67/582.2/37.2/0.373), **15.** (30, 66, 67/622.0/32.5/0.519), **16.** (30, 81, 108/632.4/45.2/0.251), **17.** (30/542.0/36.8/0.218), **18.** (43, 94/460.4/52.7/0.191), **19.** (30/425.0/51.5/0.122), **20.** (48, 56, 60,

65/416.3/67.0/0.160), **21.** (15, 41, 66/629.0/39.0/0.455), **22.** (23, 30/588.1/25.3/0.418), **23.** (30/679.4/41.5/0.322), **24.** (30/679.3/41.0/0.272), **25.** (30.577.0/44.5/0.240), **26.** (106/496.5/37.1/0.300), **27.** (10, 32, 96/466.7/36.4/0.281), **28.** (87, 101/642.0/35.0/0.306), **29.** (101/557.0/39.6/0.292), **30.** (78/523.1/30.2/0.360), **31.** (13, 91, 102/437.7/53.1/0.302), **32.** (53, 58/400.0/52.4/0.200), **33.** (12, 41/707.6/42.9/0.508), **34.** (12/723.1/42.9/0.404), **35.** 12, 41/715.6/42.9/0.562), **36.** (26/655.4/37.8/0.298), **37.** (26, 57, 105/647.0/37.8/0.340), **38.** (45, 57, 105/623.8/37.5/0.350), **39.** (26, 105/667.2/37.8/0.334), **40.** (72, 101/503.0/55.3/0.191), **41.** (4, 23, 66/530.6/30.3/0.371), **42.** (3, 6/679.0/19.2/1.024), **43.** (35, 69/510.0/63.0/0.190), **44.** (6, 7, 30, 50, 68, 86/513.9/61.4/0.644), **45.** (61/614.0/44.5/0.842), **46.** (23/531.0/30.4/0.400), **47.** (107/508.5/47.4/0.283), **48.** (46/593.0/62.8/0.510), **49.** (24, 37, 58, 100/469.0/71.9/0.206), **50.** (79, 107/546.0/33.6/0.391), **51.** (4, 23/500.2/33.7/0.336), **52.** (30, 79, 99, 107/523.2/38.3/0.377), **53.** (29, 90, 108/560.1/45.5/0.249), **54.** (18, 98/375.3/50.2/0.216), **55.** (93/408.0/65.9/0.253), **56.** (39, 95/324.7/83.1/0.133), **57.** (34/461.0/64.8/0.329), **58.** (92/554.0/47.0/0.184), **59.** (59, 91/514.3/41.0/0.368), **60.** (30, 50, 51/580.0/55.0/0.349), **61.** (7, 28, 40/512.6/80.9/0.566), **62.** (56, 79, 107/506.8/46.9/0.324), **63.** (30/692.0/36.4/0.430), **64.** (21/545.0/39.5/0.496), **65.** (2, 55/553.4/38.5/0.331), **66.** (4, 23/512.8/33.7/0.316), **67.** (107/554.4/34.8/0.382), **68.** (107/487.2/60.0/0.252), **69.** (17, 30, 42/697.6/50.1/0.443), **70.** (17, 30, 41, 24/704.6/51.5/0.505), **71.** (4, 30/645.6/42.5/0.393), **72.** (79, 107/530.6/40.0/0.350), **73.** (6, 16, 21/549.8/43.0/0.568), **74.** (6, 11, 21, 30, 76/506.2/39.7/0.614), **75.** (4/476.3/38.0/0.271), **76.** (45, 57, 89/621.0/46.0/0.299), **77.** (45, 88/645.0/46.5/0.296), **78.** (75/618.0/54.7/0.370), **79.** (30, 47, 64/588.0/63.1/0.346), **80.** (2/640.0/24.8/0.543), **81.** (3, 6, 7, 21, 30/652.5/28.6/0.594), **82.** (6, 7, 21, 97/587.7/39.1/0.579), **83.** (2, 25, 30, 55/561.0/38.3/0.344), **84.** (17, 30, 42/694.2/61.3/0.438), **85.** (6, 11, 16, 103, 104/508.4/47.6/0.664), **86.** (30, 50, 51/612.0/54.0/0.520), **87.** (30/564.4/41.8/0.313), **88.** (36, 79, 107/549.4/33.3/0.390), **89.** (22, 45, 46, 57, 63/620.0/56.3/0.240), **90.** (20, 38, 95/430.8/78.8/0.256), **91.** (61, 70, 77, 94/661.2/58.4/0.264), **92.** (101/632.0/53.0/0.224), **93.** (8, 77, 83, 94/545.0/43.0/0.217), **94.** (86/536.4/53.7/0.218), **95.** (84/346.3/37.6/0.251), **96.** (5, 52, 71, 80/647.3/221.2/0.344).

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NOTATION

T – temperature (K)

p^0 – vapor pressure (bar)

p – pressure (bar)

Greek letters

χ – polarity factor

ω – acentric factor

Subscripts

c – critical property

r – reduced property

Superscripts

(0) – simple fluid function

(1) – normal fluid correction term

(2) – polar fluid correction term

ИЗВОД

НОВЕ ВРЕДНОСТИ ФАКТОРА ПОЛАРНОСТИ

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У овом раду предложене су нове вредности фактора поларности χ за 96 супстанци. Процедура израчунавања тестирана је на вредностима овог фактора из оригиналног рада.

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