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# APPENDIX A

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## PROPERTY DATA BANK

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This appendix contains selected property values; many of these have been used to compare the methods of the text. It is limited to those pure substances for which an experimentally validated critical temperature is listed in the Thermodynamics Research Center (TRC) data bank, College Station, TX, USA, or in the other reliable sources listed below. The values have been published with permission of TRC. Not all properties are experimentally available for all substances listed, but some estimates have been made with the methods described in the main body.

The *Formula* listing for the substances has the atoms in alphabetical order except H follows C; the table has the species' formula in alphabetical order. The *Name* used is from the IUPAC as given by TRC, although we have also given common names for some substances.

Our symbols, fonts and equations are given below. The standard-state Gibbs energy and enthalpy of formation are for the species as an ideal gas at 298.15 K and 1.01325 bar (1 atmosphere). The reference states for the elements are as follows:

Ideal gases at 298.15 K and 1.01325 bar: Ar, Cl<sub>2</sub>, D<sub>2</sub>, F<sub>2</sub>, He, H<sub>2</sub>, Kr, Ne, O<sub>2</sub>, Rn, T<sub>2</sub>, Xe.

Crystalline solid at 298.15 K and 1.01325 bar: Al, As, B, C, I<sub>2</sub>, P, S, Se, Si, Ti, U

Saturated Liquid at 298.15 K: Br<sub>2</sub>, Hg

The table headings are as follows:

Section	Column Heading	Definition
All	No.	Number for this data base
All	Formula	alphabetical listing of atoms in molecule, except H follows C
All	Name	IUPAC name (common name)
All	CAS#	Chemical Abstracts Registry Number
A	Mol. Wt.	molecular weight, g mol <sup>-1</sup>
A	Tfp	atmospheric (normal) freezing/melting point, K
A	Tb	atmospheric (1.01325 bar) boiling point, K
A	Tc	vapor/liquid critical temperature, K
A	Pc	vapor/liquid critical pressure, bar
A	Vc	vapor/liquid critical volume, cm <sup>3</sup> mol <sup>-1</sup>
A	Zc	vapor/liquid critical compressibility factor = $P_c V_c / (R T_c)$

Section	Column Heading	Definition
A	Omega	Pitzer acentric factor = $-\log_{10} (P_{vp}/P_c)_{T/T_c=0.7} - 1$ (see Chap. 2)
B	DelHf0	standard state enthalpy of formation (see Chap. 3), kJ mol <sup>-1</sup>
B	DelGf0	standard state Gibbs energy of formation (see Chap. 3), kJ mol <sup>-1</sup>
B	DelHb	enthalpy change of atmospheric boiling, kJ mol <sup>-1</sup> (see Chap. 7)
B	DelHm	enthalpy change of atmospheric melting, kJ mol <sup>-1</sup>
B	V liq	liquid molar volume, cm <sup>3</sup> mol <sup>-1</sup> , at T liq
B	T liq	temperature for V liq, K
B	Dipole	molecular dipole moment, debye, $3.162 \times 10^{-25} (\text{J m}^3)^{1/2}$ (see Chap. 2)
C	T range	range of temperatures for which ideal gas heat capacity at constant pressure ( $C_p^\circ$ ) data were fitted by TRC to polynomial $C_p^\circ/R = a_0 + a_1*T + a_2*T^2 + a_3*T^3 + a_4*T^4$ with T in K. The value of $C_p^\circ$ is obtained by multiplying the result of the above equation by a value of the universal gas constant, R, and it will have the same units as the R used (see Table 2-1). Values at any temperature outside of T range are expected to be erroneous.
C	a0; a1; a2; a3; a4	parameters for TRC polynomial equation for $C_p^\circ/R$ .
C	CplG	TRC tabulated values for $C_p^\circ$ at $T = 298.15$ K or calculated from the polynomial where R has been taken as 8.3143 J mol <sup>-1</sup> K <sup>-1</sup>
C	Cpliq	TRC or other tabulated values for $C_p^\circ$ of the liquid at $T = 298.15$ K; J mol <sup>-1</sup> K <sup>-1</sup>
D	Equation #	number of equation for calculating pure vapor pressure, Pvp, bar (see Chap. 7)
	Equation #1:	$\log_{10}(Pvp) = A - B/(T + C - 273.15)$
	Equation #2:	$\log_{10}(Pvp) = A - B/(T + C - 273.15) + 0.43429x^n + E*x^8 + F*x^{12}$ where $x = (T - t_o - 273.15)/T_c$
	Equation #3:	$\ln(Pvp) = \ln(Pc) + (Tc/T)*(a*\tau + b*\tau^{1.5} + c*\tau^{2.5} + d*\tau^5)$ where $\tau = (1 - T/Tc)$
		Note: for water only the last two terms are $c*\tau^3 + d*\tau^6$
D	A/A/Tc; B/B/a; C/C/b; Tc/c; t <sub>o</sub> /d; n/Pc; E; F	parameters in Pvp Equations #1, #2, and #3. Usually A, B, C for Equation #1 are the same as those for Equation #2. Note that since Tc is a correlating parameter here, the values may differ from those in Section A.

Section	Column Heading	Definition
D	Pvpmin, bar; Tmin, K	minimum vapor pressure and temperature for an equation to be used. The minima for Equation #3 are at the triple point unless otherwise noted.
D	Pvpmax, bar; Tmax, K	maximum vapor pressure and temperature for an equation to be used. The maxima for Equation #3 are at the critical point unless otherwise noted.

Fonts have been selected to indicate the source and reliability of the values. They are as follows:

Normal (e.g., 123.45) is a value listed in the TRC data base from experiment. The data evaluation and original sources are listed in the TRC data sheets available from the Center or online at STN.

Underlined (123.45) is a value obtained from one of the references given below except a few values in section B that are from handbooks or are from the 4th Edition.

Italicized (*123.45*) is a value computed from other values in the table by the definitions given above. For  $C_p^\circ$  the TRC polynomial has been used with  $R = 8.3145 \text{ J mol}^{-1} \text{ K}^{-1}$ .

Bold (**123.45**) is an estimated value. TRC estimates some Pc values; Ambrose obtains his from the limit of Equation #3 for Pvp; other values have been estimated using methods of the main body. Steele, et al. (1996abc, 1997abcd) also estimate Tc and Pc values by fitting vapor pressure data; when both are fitted, the reliability is questionable so we have included Pc values only if the Tc was experimentally based.

Bold and italicized (***123.45***) indicates that an estimated value was used in a calculation.

Acentric factors were calculated with vapor pressure equations in Section D. Values that required an extrapolation of the Pvp equation of up to 10 K over Tmax are indicated by bold font. Values are not listed when an extrapolation of more than 10 K would have been required. When Pc is in bold font (estimated) the acentric factor is also bold.

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