Table B.2: Constants for the Antoine Equation for Vapor Pressures of Pure Species

$$\ln P^{\text{sat}}/\text{kPa} = A - \frac{B}{t/^{\circ}\text{C} + C}$$

Latent heat of vaporization at the normal boiling point  $(\Delta H_n)$ , and normal boiling point  $(t_n)$ 

		Parameters for Antoine Eqn.			Temp. Range	$\Delta H_n$	
Name	Formula	$A^{\dagger}$	В	С	°C	kJ/mol	$t_n/^{\circ}C$
Acetone	$C_3H_6O$	14.3145	2756.22	228.060	-26-77	29.10	56.2
Acetic acid	$C_2H_4O_2$	15.0717	3580.80	224.650	24—142	23.70	117.9
Acetonitrile*	$C_2H_3N$	14.8950	3413.10	250.523	<b>-27—81</b>	30.19	81.6
Benzene	$C_6H_6$	13.7819	2726.81	217.572	6—104	30.72	80.0
iso-Butane	$C_4H_{10}$	13.8254	2181.79	248.870	<b>-83—7</b>	21.30	-11.9
<i>n</i> -Butane	$C_4H_{10}$	13.6608	2154.70	238.789	-73—19	22.44	-0.5
1-Butanol	$C_4H_{10}O$	15.3144	3212.43	182.739	37—138	43.29	117.6
2-Butanol*	$C_4H_{10}O$	15.1989	3026.03	186.500	25—120	40.75	99.5
iso-Butanol	$C_4H_{10}O$	14.6047	2740.95	166.670	30—128	41.82	107.8
tert-Butanol	$C_4H_{10}O$	14.8445	2658.29	177.650	10—101	39.07	82.3
Carbon tetrachloride	$CCl_4$	14.0572	2914.23	232.148	-14-101	29.82	76.6
Chlorobenzene	$C_6H_5Cl$	13.8635	3174.78	211.700	29—159	35.19	131.7
1-Chlorobutane	C <sub>4</sub> H <sub>9</sub> Cl	13.7965	2723.73	218.265	<b>-</b> 17 <b></b> 79	30.39	78.5
Chloroform	CHCl <sub>3</sub>	13.7324	2548.74	218.552	-23-84	29.24	61.1
Cyclohexane	$C_6H_{12}$	13.6568	2723.44	220.618	9—105	29.97	80.7
Cyclopentane	$C_5H_{10}$	13.9727	2653.90	234.510	<b>-</b> 35 <b>-</b> -71	27.30	49.2
<i>n</i> -Decane	$C_{10}H_{22}$	13.9748	3442.76	193.858	65—203	38.75	174.1
Dichloromethane	$CH_2Cl_2$	13.9891	2463.93	223.240	-3860	28.06	39.7
Diethyl ether	$C_4H_{10}O$	14.0735	2511.29	231.200	-4355	26.52	34.4
1,4-Dioxane	$C_4H_8O_2$	15.0967	3579.78	240.337	20—105	34.16	101.3
<i>n</i> -Eicosane	$C_{20}H_{42}$	14.4575	4680.46	132.100	208—379	57.49	343.6
Ethanol	$C_2H_6O$	16.8958	3795.17	230.918	3—96	38.56	78.2
Ethylbenzene	$C_8H_{10}$	13.9726	3259.93	212.300	33—163	35.57	136.2
Ethylene glycol*	$C_2H_6O_2$	15.7567	4187.46	178.650	100-222	50.73	197.3
<i>n</i> -Heptane	$C_7H_{16}$	13.8622	2910.26	216.432	4—123	31.77	98.4
<i>n</i> -Hexane	$C_6H_{14}$	13.8193	2696.04	224.317	-19-92	28.85	68.7
Methanol	$CH_4O$	16.5785	3638.27	239.500	<b>-11—83</b>	35.21	64.7
Methyl acetate	$C_3H_6O_2$	14.2456	2662.78	219.690	<b>-</b> 23 <b></b> 78	30.32	56.9
Methyl ethyl ketone	$C_4H_8O$	14.1334	2838.24	218.690	-8-103	31.30	79.6
Nitromethane*	CH <sub>3</sub> NO <sub>2</sub>	14.7513	3331.70	227.600	56—146	33.99	101.2
<i>n</i> -Nonane	$C_9H_{20}$	13.9854	3311.19	202.694	46—178	36.91	150.8
iso-Octane	$C_8H_{18}$	13.6703	2896.31	220.767	2—125	30.79	99.2
<i>n</i> -Octane	$C_8H_{18}$	13.9346	3123.13	209.635	26—152	34.41	125.6
<i>n</i> -Pentane	$C_5H_{12}$	13.7667	2451.88	232.014	-4558	25.79	36.0
Phenol	$C_6H_6O$	14.4387	3507.80	175.400	80—208	46.18	181.8
1-Propanol	$C_3H_8O$	16.1154	3483.67	205.807	20—116	41.44	97.2
2-Propanol	$C_3H_8O$	16.6796	3640.20	219.610	8—100	39.85	82.2

Table B.2	(Continued)
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		Parameters for Antoine Eqn.			Temp. Range	$\Delta H_n$	
Name	Formula	$A^{\dagger}$	В	С	°C	kJ/mol	$t_n$ /°C
Toluene	$C_7H_8$	13.9320	3056.96	217.625	13—136	33.18	110.6
Water	$H_2O$	16.3872	3885.70	230.170	0-200	40.66	100.0
o-Xylene	$C_8H_{10}$	14.0415	3358.79	212.041	40—172	36.24	144.4
<i>m</i> -Xylene	$C_8H_{10}$	14.1387	3381.81	216.120	35—166	35.66	139.1
<i>p</i> -Xylene	$C_8H_{10}$	14.0579	3331.45	214.627	35—166	35.67	138.3

Based primarily on data presented by B. E. Poling, J. M. Prausnitz, and J. P. O'Connell, *The Properties of Gases and Liquids*, 5th ed., App. A, McGraw-Hill, New York, 2001.

<sup>\*</sup>Antoine parameters adapted from J. Gmehling, U. Onken, and W. Arlt, *Vapor-Liquid Equilibrium Data Collection*, Chemistry Data Series, vol. I, parts 1–8, DECHEMA, Frankfurt/Main, 1974–1990.

<sup>&</sup>lt;sup>†</sup>Antoine parameters A are adjusted to reproduce the listed values of  $t_n$ .