Websites

EPA Estimation Program Interface (EPI) Suite. Estimation for octanol–water partition coefficient log K_{ow}, Henry's law constant, melting point, boiling point, vapor pressure, water solubility. Requires SMILES notation with help guide. http://www.epa.gov/oppt/exposure/docs/episuite.htm.

Exercises

1. Develop correlations for the van der Waals attraction term a and the volume term b, using the molecular weight as the predictor.

   (a) Find the values of a and b for the following families of compounds: noble gases, period 1 to 6; normal paraffins, 1 to 20 carbon atoms; 1-chloro paraffins, 1 to 10 carbon atoms; 1-alcohols, 1 to 10 carbon atoms.
   (b) Make graphs of van der Waals a (y axis) versus MW (x axis). How do these four families differ in their intercepts and slopes? Which chemical has the largest slope (most molecular weight dependent), and which chemical has the smallest slope?
   (c) Make one-parameter linear correlations and compute their R^2 and SD values.

2. Make a correlation for the viscosity of R134a in μPa s, from −50 to +100 °C in 10 °C intervals. (Hint: a possible source of data is NIST Chembook.)

   (a) Make a linear regression in the form $\mu = C_0 + C_1 T$. Obtain the coefficients C_0 and C_1, as well as R^2, SD$(\mu - \mu')$, the maximum error, and the maximum percentage error.
   (b) Make a more accurate quadratic regression in the form $\mu = C_0 + C_1 T + C_2 T^2$. Compare the improvements of the quadratic correlation on the values of R^2, the standard error, the maximum error, and the maximum percentage error.
   (c) Make an exponential regression in the form $\mu = C_0 \exp(C_1 T)$. How does it compare with the two previous correlations?

3. The correlations of liquid viscosities with structural and ambient parameters pose difficult problems. Yaws recommended the following equation for the viscosity at 25 °C for paraffins:

$$\log_{10}(\mu) = A + B/T + CT + DT^2 \quad T \text{ in kelvin}$$

   The recommended parameter values, and the temperature range of validity, are:

   (a) Make plots of viscosity versus temperature in the range −50 °C (coldest winter in North America) to 250 °C (hot engine) for these six compounds.

(b) If the DT^2 term is eliminated, how much difference would it make to the results?

	A	B	10^2C	10^5D	*Min. T*	*Max. T*
C_6	−5.0715	655.36	1.2349	−1.5042	178	507
C_8	−5.9245	888.09	1.2955	−1.3596	216	569
C_{10}	−6.0716	1017.7	1.2247	−1.1892	243	618
C_{12}	−7.0687	1253.0	1.3735	−1.2215	262	658
C_{14}	−7.8717	1446.7	1.4940	−1.2495	260	692
C_{16}	−8.1894	1557.0	1.5270	−1.2371	291	721

4. The Joule–Thompson coefficient measures the temperature change when a gas is expanded into a vacuum. For the refrigerant R134a, we have the following values:

Temperature, °C	*Joule–Thomson coefficient × 10^5, K/torr*
−50	−4.19
−40	−3.92
−30	−3.61
−20	−3.24
−10	−2.79
0	−2.26
10	−1.60
20	−0.770
30	0.297
40	1.71
50	3.66
60	6.48
70	10.9
80	18.6
90	35.9
100	109.3

(a) Make a plot of the Joule–Thompson coefficient versus temperature. What functional form would you suggest that would require the least number of coefficients to achieve the highest value of R^2?

(b) Make the correlation; compute the values of R^2, standard error, maximum error, and maximum percentage error.