

## ERRATTA

Air-Water Partition Coefficient - Chapter 8

Concepts and Theory of Chemical Property Estimation - Chapter 2

Diffusivity - Chapter 12

Octanol-Water Partition Coefficient - Chapter 9

Soil and Sediment Sorption Coefficient - Chapter 10

CONCEPTS AND THEORY OF CHEMICAL PROPERTY ESTIMATION - CHAPTER 2

**Page 11, paragraph 1, line 4, Eqn. 2.2**

*Now reads*  $\Delta G = \Delta H + T\Delta S$

*It should read*  **$\Delta G = \Delta H - T\Delta S$**

AIR WATER PARTITION COEFFICIENT - CHAPTER 8

**Page 123, paragraph 1, line 10**

*Now reads* .....where  $V_{ml}$  ( $\text{mol}/\text{m}^3$ ) is the molar volume....

*It should read* .....where  $V_{ml}$  ( $\text{m}^3/\text{mol}$ ) is the molar volume...

**Page 130, paragraph 1, line 4, Eqn 8.10**

*Now reads*  $\log K_{AW} = \sum_i a_i g_i + \sum_j b_j F_j$

*It should read*  **$\log g = \sum_i a_i g_i + \sum_j b_j F_j$ ;  $1/g = K_{AW}$**

Meylan and Howard's model directly estimates  $1/K_{AW}$ .

**Page 130, Example**

*Now reads* .... $\log K_{AW} = \sum_i a_i g_i + \sum_j b_j F_j$

$$= (7)(-0.1197) + (2)(0.2326) + (1)(1.0855) + (1)(3.2301) + (1)(-0.20) \dots$$

*It should read* ..... **$\log g = \sum_i a_i g_i + \sum_j b_j F_j$**

$$= (7)(-0.1197) + (2)(0.1163) + (1)(1.0855) + (1)(3.2301) + (1)(-0.20)$$

$$= 3.5112$$

The measured value of  **$\log g = \log 1/K_{AW}$**  is 3.55.....

**Page 131, Table 8.2**

*The title now reads* Bond Contribution to Log  $K_{AW}$  at 25EC

*It should read* **Bond Contribution to Log  $g$  at 25EC. See Equation 8.10**

**Page 132, Table 8.3**

*The title now reads* Correction Factors for Log  $K_{AW}$  at 25EC

*It should read* **Correction Factors for Log  $g$  at 25EC. See Equation 8.10**

OCTANOL-WATER PARTITION COEFFICIENT - CHAPTER 9

**Page 139, Example**

*Now reads*

1. Identify the significant fragments found in the molecular structure.

The structure contains four CH<sub>3</sub>, two CH<sub>2</sub>, two -C\*H<, one >C\*<.....

*It should read*

**1. Identify the significant fragments found in the molecular structure.**

**The structure contains four CH<sub>3</sub>, two CH<sub>2</sub>, three -C<sub>r</sub>H<, three =C<sub>r</sub><.....**

**PAGE 142, EXAMPLE**

*Now reads*  $\log K_{OW} = a + \sum_i b_i B_i + \sum_j c_j C_j$

$$= -0.703 + (4)(0.661) + (2)(0.415) + (2)(0.104) + (3)(0.380) + (1)(0.129) + (1)(0.135) \\ = 4.25$$

The measured value of  $\log K_{OW}$  is 4.36. The estimate error is 2.6%.....

*It should read*  $\log K_{OW} = a + \sum_i b_i B_i + \sum_j c_j C_j$

$$= -0.703 + (4)(0.661) + (2)(0.415) + (2)(0.104) + (3)(0.380) + (3)(0.129) + (1)(0.135) \\ = 4.51$$

**The measured value of  $\log K_{OW}$  is 4.36. The estimate error is 3.4%.....**

**Page 197, EXAMPLE**

3. If we assume that sorption is a linear function of solute concentration,  $K_P = K_d = f_{OC} K_{OC}$

$$\text{or } K_{OC} = K_P / f_{OC}$$

$$\log K_{OC} = \log K_P - \log f_{OC} \\ = 3.21 - \log 0.0270 \\ = 4.78$$

**Page 200, paragraph 1**

This paragraph concerns  $K_P$  values, not  $K_{OC}$  values. *It should read* **A**.....The estimate of  $\log K_P$  is in error by 40%. However, the  $\log K_P$  value of pentachlorophenol...

**DIFFUSIVITY - CHAPTER 12**

**Page 250, Example**

*Now reads* Estimate the diffusivity in air of carbon tetrachloride, CCl<sub>4</sub>, at 25°C and 1 atm pressure...

*It should read* **Estimate the diffusivity in air of carbon tetrachloride, CCl<sub>4</sub>, at 25°C and 1 bar pressure...**