

Table 7.3 Equations for Prediction of Water Solubility

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Fundamental equations

liquid solutes

$$\log S_w = -1.072 \log PC + 0.672$$

crystalline solutes: rigid nonelectrolyte drug molecules

$$\log S_w^c \approx -\log PC - 0.01 MP + 1.05$$

Applied equations

rigid polycyclic aromatic hydrocarbons, e.g., naphthalene

$$\log S_w^c = -0.88 \log PC - 0.01 MP - 0.012$$

mono- and multifunctional halobenzenes, e.g., 1,2-dichlorobeneze

$$\log S_w^c = -0.99 \log PC - 0.01 MP + 0.72$$

steroid hormones, e.g., progesterone

$$\log S_w^c = -0.88 \log PC - 0.01 MP + 0.08$$

hexamethylmelamines, e.g., hexamethylmelamine

$$\log S_w^c = -0.904 \log PC - 0.007 MP + 0.07$$

alkyl *para*-substituted benzoates, e.g., hexyl-*p*-aminobenzoate

$$\log S_w^c = -1.14 \log PC - 0.005 MP + 0.633$$

alkyphenols

$$\log S_w^c = -0.997 \log PC - 0.008 MP + 1.43$$

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Source: From Ref. 9.