Qualitative understanding of partition preferences

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- ↓ 🛛 🔵 Answer
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10) Evaluation of the software PcKocWIN

Question:

PcKocWIN is a software that calculates the log $K_{ioc/water}$ -values of compounds whose chemical structure is entered in SMILES notation. This program is made available by the US-Environmental Protection Agency on their web site (http://www.epa.gov /oppt/exposure/docs/episuitedl.htm).

PcKocWIN calculates benzene and phenol (in its non-ionic form) to have identical log K -values. Is this plausible?

For polar compounds like ethanol, ethanediol and others this software calculates negative log $K_{i \text{ oc/water}}$ -values that are subsequently corrected to a value of zero (i.e. $K_{i \text{ oc/water}} = 1 (L_{water / kg \text{ oc}})$) because this is believed to be the lower limit of possible log $K_{i \text{ oc/water}}$ -values. In the case of ethanediol the difference between the adjusted and the non-adjusted log K i oc/water -value amounts to more than one order of magnitude. What do you think about this?

Output of PcKocWIN for ethanediol HO-CH, -CH, -OH

Koc (estimated): 1 SMILES : OCCO CHEM : 1,2-Ethanediol MOL FOR: C2 H6 O2 MOL WT : 62.07

----- PCKOCWIN v1.66 Results -----

You will have to check your answer to this question by yourself ...

