10) Evaluation of the software PcKocWIN

Question:

PcKocWIN is a software that calculates the log $K_{i\,oc/water}$ -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 $K_{i\,oc/water}$ -values. Is this plausible?

For polar compounds like ethanol, ethanediol and others this software calculates negative log $K_{i\,oc/water}$ -values that are subsequently corrected to a value of zero (i.e. $K_{i\,oc/water} = 1$ ($L_{water\ /kg\ oc}$)) because this is believed to be the lower limit of possible log $K_{i\,oc/water}$ -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_2 -CH_2 -OH

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

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

First Order Molecular Connectivity Index ..... : 1.914
Non-Corrected Log Koc ..... : 1.6414
Fragment Correction(s):
2 Aliphatic Alcohol (-C-OH) ..... : -3.0386
Corrected Log Koc ..... : **-1.3972**
Over Correction Adjustment to Lower Limit Log Koc ... : **0.0000**
Estimated Koc: 1

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