Quantitative prediction of K values

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Problem 3

a) Calculate the $K_{oc/water}$ values of phenol and benzene with the software KOCWIN^{TM} supplied by U.S. EPA. Compare and discuss the results.

Answer:
Phenol is a highly bipolar compound while benzene is not. This should typically result in very different partition behaviour unless the two phases in the partition system are almost identical in their polarity. The latter is certainly not the case with water and soil organic matter, hence, different K_{oc} values should be expected.

b) Calculate the $K_{oc/water}$ value of 1,2-ethanediol with KOCWIN^{TM} and discuss the result.

Answer:
In all cases where KOCWIN^{TM} does calculate a negative log K_{oc} value (i.e. a K_{oc} value smaller than 1) this value is deliberately corrected to 0 by the software (i.e. K_{oc} = 1). It is not clear why this is done but it is definitely clear that negative log K_{oc} values are realistic for highly polar organic compounds (i.e., these compounds prefer the water phase over the soil organic carbon phase) so that this correction is not justified.