5) Interpretation of data taken from a publication

Question:

Partitioning data for air-water and octanol-water were listed in a publication as in the table below. The values were not defined as K_{aw} and K_{wa} or K_{ow} and K_{wo}. Can you tell even without this information?

chemical	Air-water partitioning	Octanol-water partitioning
Heptane	0.011	32000
Phenol	70800	29
Chlorobenzene	6.6	776

Answer:

The compounds are roughly similar in size. Hence, differences in the cavity energy will likely not be the cause for the observed differences in the partitioning. Thus, only the direct interactions between the solute molecules and the phase molecules can explain these differences. Due to its H-bond interactions, phenol will like the water phase much more than heptane does. Hence, one can conclude that the air-water partition constants are defined as K_{wa} . Along the same line of reasoning on can conclude that the octanol-water data are defined as K_{ow}.