## Qualitative understanding of partition preferences

- Introduction
- Cavity model
- Rules for partitioning
- The cavity model in quantitative terms

## ▼ Selftest

- ↓ 1) What does the cavity model say?
- ↓ Answer
- ↓ **0** 2) Main interactions ... ?
- ↓ 🛛 🔍 Answer
- ↓ 3) Size of a *solute* molecule ... ?
- \downarrow 🛛 🔍 Answer
- ↓ 4) Size of the *solvent* molecule ... ?
- ↓ Answer
- ↓ 5) Interpretation of data
- 🕴 🍳 Answer
- ↓ 6) "Like dissolves like"
- ↓ Answer
- ↓ 0 7) Concept maps
- ↓ 8) Functional groups
- ↓ Answer
- ↓ 9) Illustration by given data?
- ↓ Answer
- ↓ 10) Evaluation of the software PcKocWIN
- ↓ 11) H-bonds between given substances?
- ↓ 12) Tendency to distribute
- ↓ Answer
- ↓ 13) Gas chromatography
- ↓ Answer
- ↓ 14) Henry's Law constant
- ↓ Answer
- \downarrow 🌔 15) Quiz
- Problems
- Intermolecular interactions in every day life
- FAQ

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

5) Interpretation of data taken from a publication

## Answer:

**Ouestion:** 

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 Kow.

