The cavity model in quantitative terms

The animation below gives you a more quantitative idea about how different interaction energies contribute to the overall partitioning constant. These are only rough calculations but they give a good idea of the absolute strength of various interactions. The partitioning between two liquid phases is typically dominated by H–bond interactions. But it would be erroneous to conclude from this that van der Waals interactions are weak compared to H–bond interactions. They are in fact much stronger for almost all molecules but in liquid/liquid partitioning these contributions largely cancel and thus do not become "visible". Therefore, the animation only shows air/solvent partitioning. Of course, you can easily deduce liquid/liquid partition data from combining the data from the two air/liquid partition systems for the respective liquids.
More details on the quantitative estimation of partition constants are given in the next chapter.

Calculating solvent/air partitioning from interaction energies

	Molecule 1			Molecule 2		
Volume (cm³/mol)	30 60 90 120 150			30 60 90 120 150		
H-donor (rel. units)	0 0.2 0.4 0.6 0.8			0 0.2 0.4 0.6 0.8		
H-acceptor (rel. units)	0 0.2 0.4 0.6 0.8			0 0.2 0.4 0.6 0.8		

Energies (in kJ/mol)

- VdW
- cavity
- H-bond

	Solvent			Solvent		
	Hexane	Ethanol	Water	Hexane	Ethanol	Water
Total free energy	-4.81	-2.61	3.38	-4.81	-2.61	3.38
$K_{solvent/air}$	6.97	2.87	0.256	6.97	2.87	0.256

Choose the molar volume and the H-bond-donor and H-bond-acceptor properties of a fictional molecule and watch the interactions energies in various solvents change as well as the corresponding solvent/air partition constant. (Note: the numbers that appear below are only rough estimates).

Here are some typical values for your orientation:
molar volume in cm³/mol: 45 ethanol, 72 benzene, 145 phenantrene
H-bond acceptor (rel. units): 0 alkanes, 0.1-0.2 for conjugated double bonds, 0.45 for the oxygen in ethers, aldehydes, esters, ketones, alcohols.
H-bond donor (rel. units): 0 alkanes, 0.4 for the proton in an –OH group.