Problem 4

Your task is to check whether two polymers of unknown origin do possess similar sorption properties at 15°C. In order to limit your efforts, you are advised to measure air/polymer partitioning for only five different compounds. What type of compounds would you use? Which criteria do these compounds have to fulfill?

Answer:
The compounds must be as diverse as possible with respect to the different types of interaction: There should be two compounds that do not have any polar interactions but that differ in their van der Waals interaction energy, e.g. pentane and nonane. Then there should be a monopolar H-bond acceptor with a small S-descriptor such as diethylether. Additionally, there should be a strong H-bond donor such as an alcohol (unfortunately there are no strong monopolar H-bond donors). And eventually, there should be a compound with a high S-descriptor and as low as possible A and B-descriptors, e.g. naphthalene.