Qualitative understanding of partition preferences

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FAQ

5) How does a mixture of similar isomeres behave?

Question:

How does a mixture of similar isomeres (e.g. alkanes with the same number of C Atoms but differently branched: n-octane, 2,2,4trimethylpentane, 2-propylpentane, 2-ethyl-3-methylpentane) behave regarding its saturation vapour pressure, solubility in water and other aspects of partitioning?

Does it behave a) like a mixture of many separate compounds or b) like one compound?

Answer:

The answer becomes clear if we look at an extreme case: the partitioning of different compounds that possess identical partition properties. In this case it does not make any difference whether we treat the compounds as separate compounds with separate concentrations c_1 , c_2 , and c_3 and separate partition constants K_1 , K_2 , K_3 (which are of course all the same) or if we treat them as a single compound with $c_{tot} = c_1 + c_2 + c_3$ and $K = K_1 = K_2 = K_3$. The results will be exactly the same. Isomers like the branched alkanes in the above question will have similar (but not identical partition properties). For many purposes it may suffice to treat them as one compound (especially if we don't know all the individual partition constants). But if the differences happen to matter then they should be treated as separate compounds.

