Which organic compounds has the highest potential to bio-accumulate in aquatic life?

A. Decane B. Toluene **C. Stearic acid** D. 1-Decanol

This estimation is based on the octanol-to-water partition coefficient, k_{ow}, which is the ratio between a compound's solubility in octanol to its solubility in water.

$$k_{ow} = \frac{[\text{analyte}]^{\text{octanol phase}}}{[\text{analyte}]^{\text{aqueous phase}}}$$

Chemicals with low k_{ow} values (e.g., less than 10) may be considered relatively hydrophilic; they tend to have high water solubilities, small soil/sediment adsorption coefficients, and small bioconcentration factors for aquatic life. Conversely, chemicals with high k_{ow} values (e.g., greater than 10^4) are very hydrophobic.[1] In short, the higher the k_{ow}, the more likely the analyte will participate in the organic phase, ie. it will be more lipophilic in water, so that it will tend to dissolve in animals' lipids more preferably than water.[2]

As a general rule, saturated hydrocarbons usually have high tendency to participate into the organic layer since water won't dissolve them.

Usually acids have low k_{ow} values however, stearic acid has 18 carbons and it'ns saturated hydrocarbon chain is a lot longer than decane. Stearic acid is used in a lot of things like soap bars (to retain their shapes) and facial cleansers and thus will persist in aquatic environments. Luckily stearic acid is a naturally occurring product and relatively harmless but this idea is important to keep in mind when designing new compounds with potential toxicity.

1. https://www.pirika.com/ENG/TCPE/logP-Theory.html
2. The octanol-to-water partition coefficients can be either estimated using this program: www.vcclab.org/lab/alogps/start.html
   Or estimated using chemdraw (detailed calculation methods can be found in this book)
   "Physical-Chemical Properties and Environmental Fate for Organic Chemicals"
   http://rushim.ru/books/spravochniki/mackay1.pdf