

Quantitative prediction of K values

- Introduction
- Fragment models
 - sp-LFERs
 - pp-LFERs
 - Comparison of the various methods
 - Predictive models based on molecular structure
- Critical remarks on approaches from chemical engineering

▶ Selftest

▼ Problems

- ↓ ● Problem 1
- ↓ ● **Problem 2**
- ↓ ● Problem 3
- ↓ ● Answer
- ↓ ● Problem 4
- ↓ ● Answer
- ↓ ● Problem 5
- ↓ ● Answer
- ↓ ● Problem 6
- ↓ ● Answer
- ↓ ● Problem 7
- ↓ ● Problem 8
- ↓ ● Problem 9

Problem 2

a) Why is the order of compound classes in the figure below (from page "Single-parameter Linear Free Energy Relationships") in the plot "ethanediol vs. octanol" almost opposite to the one in "hexadecane vs. olive oil" and "olive oil vs. octanol" (olive oil is an ester)?

b) And why are the slopes so shallow in the "ethanediol vs. octanol" plot?

Your knowledge from Chapter 4 will help you to answer these questions.

