

## 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
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- ↓ ● Problem 5
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- ↓ ● **Problem 9**

## Problem 9

The US Environmental Protection Agency recommends on one of their websites that –if in doubt– experimental partition constants are to be preferred over predicted ones. Do you agree?

