

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

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Question 1

Fragment models (textbook V.1) are based on the assumption that a specific molecular fragment (e.g. $-\text{CH}_2$ or $-\text{OH}$) always contributes the same incremental value to the logarithm of a specific partition constant, no matter in which molecular surrounding they occur.

Find examples for and against this assumption in the data of file [Kaw.xls](#) for the following molecular increments: $-\text{OH}$, $-\text{Cl}$ and $-\text{CH}_2$.

