

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
- ↓ ● Question 1
 - ↓ ● Question 2
 - ↓ ● Answer
 - ↓ ● **Question 3**
 - ▶ Problems

Question 3

Use the data from the table [Kaw_increment.doc](#) to calculate the air/water partition coefficients of:

(i) toluene, chlorobenzene, benzaldehyde and nitrobenzene starting from **benzene** whose experimental $\log K_{\text{air/water}}$ is **-0.63** (L/L) at 25°C

Compound	Increment method / $\log K_{\text{aw}}$	Experimental data / $\log K_{\text{aw}}$
benzene	not applicable	-0.63
toluene		-0.65
chlorobenzene		-0.82
benzaldehyde		-2.95
nitrobenzene		-3.02

(ii) and of 2-nitrophenol, 4-nitrophenol, 2-chlorophenol and 4-chlorophenol, starting from **phenol** whose experimental $\log K_{\text{air/water}}$ is **-4.85** (L/L) at 25°C.

Compare the results with the experimental values.

Compound	Increment method / $\log K_{\text{aw}}$	Experimental data / $\log K_{\text{aw}}$
phenol	not applicable	-4.85
2-nitrophenol		-3.36
4-nitrophenol		-7.81
2-chlorophenol		-3.34
4-chlorophenol		-5.16

