

## Empirical method for calculation properties of organic substances and chemical similarity recognition

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### Abstract

Empirical method for pK(a) prediction based on LFER, experimental solvent properties and atomic contributions shows good accuracy and universality. Values of involved empirical parameters make possible to discriminate organic acids by type of the protonation centre.

**Keywords:** Empirical method; Atomic contributions; pK(a); Properties estimation; Chemical similarity

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