

# Improved QSAR Analysis of the Toxicity of Aliphatic Carboxylic Acids<sup>1</sup>

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**Abstract** - The results of a QSPR study of the toxicity of carboxylic acids in aqueous solution are reported. The molecular set comprises 35 carboxylic acids with the corresponding  $pK_a$  values in water. The set of molecular and topological parameters includes electrotopological state of the carboxy and methyl groups, molar refractivity, refractive index, *n*-octanol–water partition coefficient  $\log K_{o/w}$ , surface tension, and polarizability. Quite reasonable estimates are obtained, which improve the results of previous theoretical calculations.