QSPR Model for the Dielectric Constant of Fatty Acids

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The dielectric constant, or permittivity (ϵ), is a dimensionless constant that indicates how easy a material can be polarized by imposition of an electric field on an insulating material. This property is in general influenced by temperature, moisture levels, and electrical frequency. The effect of temperature on the dielectric constant provides information about association. For saturated fatty acids, the extent of association increases with the number of carbon atoms in the molecule. Furthermore, with highly associated molecules, the dielectric constant increases with temperature and unsaturation due to the breaking up of the complexes. In this work a QSPR (Quantitative Structure-Property Relationships) equation is proposed to predict the dielectric constant for fatty acids:

 ϵ =3.9473(n^- 0.201) + 1.492E-6(T-344)EXP(-0.3767n)

ε=2.361 + 0.223db - 1.0E-4(1.359 - 8.705db)(T-273)

In these equations *T*, *n* and db represent the temperature (K), the carbon atoms, and db double bonds at *n*=18. The ε_{cal} figures were calculated and compared to the experimental measurements from literature over temperature ranges (293-393 K). The proposed QSPR model predicts acceptable values for ε with average error 0.97 % for the equation ε =f(n,T) and -1.33 % for ε =f(db,T).