

## A QSPR Correlation for Dielectric Constant

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The dielectric constant (DC) or relative static permittivity of a material represents the electrical capacitance of the material relative to that of a vacuum and is important in many industrial applications. DC values are a recent addition to the DIPPR<sup>®</sup> 801 pure chemical database. The task of providing reliable DC values for all compounds in the database is a challenge because of the paucity of experimental values and the unreliability of current prediction methods. Available DC prediction methods are rather rudimentary and often fail significantly (with errors of 100 % or more) for strongly polar compounds. As DC is directly related to molecular charge distribution and polarizability, a new QSPR (quantitative-structure-property-relation) correlation for DC has been developed using molecular descriptors available in the DIPPR<sup>®</sup> 801 database. Tests of the correlation suggest an uncertainty of less than 20 % for a wide range of organic compounds with DC values ranging from 1.0 to 50.0. The correlation requires a value of the dipole moment (DM), a property for which experimental values are also not always available. However, DM can be generated as a molecular descriptor, and we show that values obtained from density functional calculations using B3LYP/6-311+G(3df,2p) calculations can be used in the DC correlation with little decrease in accuracy of the predicted values. This permits population of nearly all missing DC values in the DIPPR<sup>®</sup> 801 database with relatively reliable predicted values.