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QSPR Modeling of the logK_{ow} and logK_{oc} of Polymethoxylated, Polyhydroxylated Diphenyl Ethers and Methoxylated-, Hydroxylated-Polychlorinated Diphenyl Ethers

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Highlights

- The structural parameters of all tested DEs were calculated by Gaussian 09
- Satisfactory QSPR models were established to predict logK_{ow} and logK_{oc} of DEs
- $N_{2(6)}$, $N_{3(5)}$ and N_4 are key factors of logK_{ow} and logK_{oc} of PMeODEs and PHODEs