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QSPR Modeling of the $\log K_{ow}$ and $\log K_{oc}$ 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 $\log K_{ow}$ and $\log K_{oc}$ of DEs
- $N_{2(6)}$, $N_{3(5)}$ and N_4 are key factors of $\log K_{ow}$ and $\log K_{oc}$ of PMeODEs and PHODEs

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