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Mostar Type Indices and QSPR Analysis of Octane Isomers

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Abstract : Chemical Graph Theory (CGT) is the branch of mathematical chemistry in which molecules are modeled to study their physicochemical properties using molecular descriptors. Amongst these descriptors, topological indices play a vital role in predicting the properties by defining the graph topology of the molecule. Recently, the bond-additive topological index known as the Mostar index has been proposed. In this paper, we compute the Mostar-type indices of octane isomers and use the data obtained to perform QSPR analysis. Furthermore, we show the correlation between the Mostar type indices and the properties.

Keywords : chemical graph theory, mostar type indices, octane isomers, qspr analysis, topological index
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