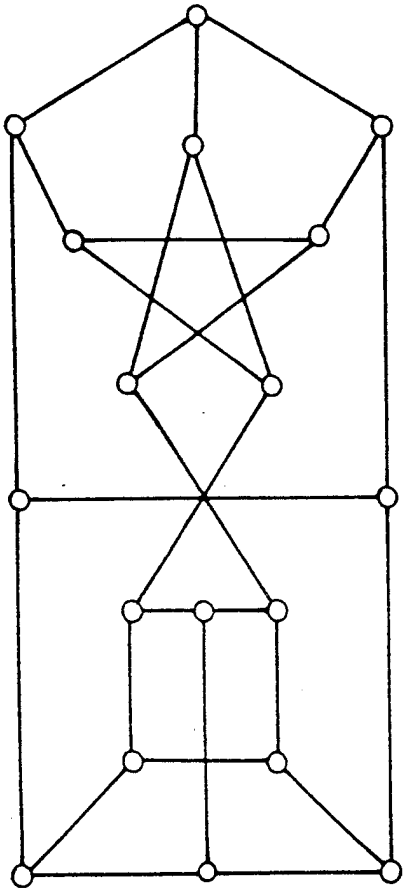
MATH/CHEM/COMP 1990

THE FIFTH INTERNATIONAL COURSE AND CONFERENCE ON THE INTERFACE BETWEEN MATHEMATICS, CHEMISTRY AND COMPUTER SCIENCE



ABSTRACTS
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MODELING OF PARTITION COEFFICIENT

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We use graph-theoretical approach to modeling of 1-octanol/water partition coefficient. Forty graph-theoretical indices were tested. The best one variable equation was obtained with first-order valence connectivity index. The power of the model is demonstrated by the accurate estimation of logP for different type of molecule. The method is easy to use and it has general applicability.