OEState

Summary

This is older C++ implementation of EState descriptors which has been used in ALOGPS program as well as in a number of publications by Dr. Igor Tetko and his co-authors. Compared to EState the OEState also includes few non E-state descriptors. Moreover, OEstate uses its own aromaticity detection.

Descriptors

See EState section, the same both atom and bond types are included

ACCEPTORS -- number of hydrogen bond acceptors
HALOG -- number of halogen atoms
MW -- molecular weight
NA -- number of heavy (all except hydrogen) atoms
NH -- number of hydrogen atoms
N -- number of nitrogen atoms
O -- number of oxygen atoms
P -- number of phosphor atoms
S -- number of sulfur atoms
PSA -- polar surface area calculated according to Peter Ertl et al algorithm
RBONDS -- number of rotatable bonds

Options

COUNTS -- If checked, instead of values of E-state the numbers of atoms and bonds having particular types of E-state index will be used. Thus, this option will force to E-state be used as fragment-like descriptors.

Reference

- Tetko, I.V.; Tanchuk, V.Yu.; Villa, A.E.P. Prediction of n-Octanol/Water Partition Coefficients from PHYSPROP Database Using Artificial Neural Networks and E-state Indices, J. Chem. Inf. Comput. Sci., 2001, 41, 1407-1421, PUBMED