ALogPS

It calculates two descriptors provided by ALOGPS program:

- ALogPS_logP -- octanol/water partition coefficient. The algorithm was developed with 12908 molecules from the PHYSPROP database using 75 E-state indicies. 64 neural networks were trained using 50% of molecules selected by chance from the whole set. The logP prediction accuracy is root mean squared error rms=0.35 and standard mean error s=0.26 [1,2].
- ALogPS_logS -- solubility in water. It was developed using 1291 molecules and provided improved aqueous solubility prediction (rms=0.49, s=0.38) compared to our previous analysis [3]. The molecules used in this study can be downloaded.

References

1. Tetko, I. V.; Tanchuk, V. Y. Application of associative neural networks for prediction of lipophilicity in ALOGPS 2.1 program, J. Chem. Inf. Comput. Sci., 2002, 42, 1136-45.
2. Tetko, I. V.; Tanchuk, V. Y.; Villa, A. E. 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, 1407-21.
3. Tetko, I. V.; Tanchuk, V. Y.; Kasheva, T. N.; Villa, A. E. Estimation of aqueous solubility of chemical compounds using E-state indices, J. Chem. Inf. Comput. Sci., 2001, 41, 1488-93.