

drug-logS

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Thanks for your interest of the solubility prediction model. The estimation of aqueous solubility was solely based on simple atom contribution. The contribution coefficients of different atom types and correction factors were generated based on a multiple linear regression using a learning set consisting of 1708 organic compounds.

I agree to use the model for research purpose only. I will not transfer or redistribution this model to other laboratories. I agree that any public reports or publication of results obtained using the prediction model of solubility will acknowledge its use by an appropriate citation (*J. Chem. Inf. Comput. Sci.* 2004, 44, 266-275 & *J. Chem. Inf. Model.* 2007, 47, 1395-1404). This license agreement is only used for user record, and no signature is necessary. Please fill the following user information, and sent it back by email to admeteam@hotmail.com

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