$ClogP_{alk}$

Introduction

$ClogP_{alk}$ is a method for predicting alkane/water log and the program is run as follows (optional commands in parentheses):

ClogPalk --help (to get help)

ClogPalk -i Structure.File -o Output.File -p parameter.File (-v Vector.Binding.File)

Structure files

$ClogP_{alk}$ needs 3D coordinates in order to calculate molecular surface area (MSA). In the 2013 JCAMD study 3D structures were generated (single conformation) from SMILES using OMEGA and these were minimised using SZYBKI (MMFF94S).

Parameter File

There are three types of parameter in the parameter file, an example of which is provided as part of the supporting information.

ref (defines reference equation that relates saturated hydrocarbon $logP_{alk}$ to MSA)
ref slope intercept

fgroup (functional group term)
fgroup SMARTS.Definition slope intercept

interaction term (interaction term)
interact SMARTS.Definition interaction.term

Vector Bindings

An optional file of vector bindings can be used both in profiling and filtering and the format of this file is as follows (with comments specified using # as first character on the line):

Vector.Binding.Name Vector.Binding.Definition

References

1. Kenny PW, Montanari CA, Prokopcyk IM (2013) $ClogP_{alk}$:A method for predicting alkane/water partition coefficient; JCAMD 27:*-* (If citing please consult journal for page numbers)

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