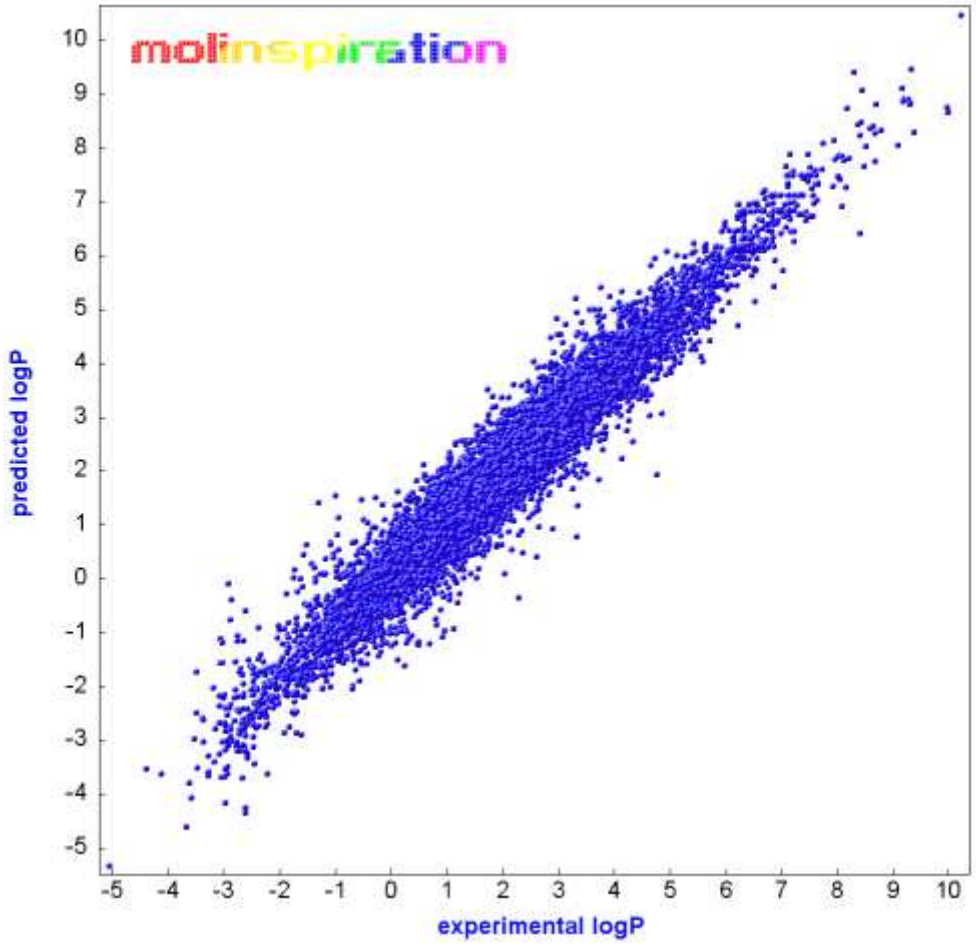
logP - octanol-water partition coefficient

Interactive logP calculator Try our logP predictor, which allows also calculation of other molecular properties including PSA, Rule of 5 parameters and molecular drug-likeness. Contact Molinspiration if you would be interested to install our logP calculation software including Molinspiration desktop property calculator locally at your site.

Octanol-water partition coefficient logP is used in QSAR studies and rational drug design as a measure of molecular hydrophobicity. Hydrophobicity affects drug absorption, bioavailability, hydrophobic drug-receptor interactions, metabolism of molecules, as well as their toxicity. LogP has become also a key parameter in studies of the environmental fate of chemicals.

Method for logP prediction developed at Molinspiration (miLogP2.2 - November 2005) is based on group contributions. These have been obtained by fitting calculated logP with experimental logP for a training set more than twelve thousand, mostly drug-like molecules. In this way hydrophobicity values for 35 small simple "basic" fragments have been obtained, as well as values for 185 larger fragments, characterizing intramolecular hydrogen bonding contribution to logP and charge interactions.
Molinspiration methodology for logP calculation is very robust and is able to process practically all organic and most organometallic molecules.



n = 12'202, r^2 = 0.944, r = 0.972, stdev = 0.428, mae = 0.328

For 50.5% of molecules logP is predicted with error < 0.25, for 80.2% with error < 0.5 and for 96.5% with error < 1.0. Only for 3.5% of structures logP is predicted with error > 1.0.
The statistical parameters listed above rank Molinspiration miLogP as one of the best methods available

for logP prediction.

Several our customers reported very good correlation between Molinspiration calculated logP and various drug transport properties. MiLogP is used due to its robustness and good prediction quality in the popular ZINC database for virtual screening. A report by National Institute of Standards documenting excellent agreement between experimental logP and Molinspiration calculated logP for some industrial chemicals is available on-line.

Additional information about other properties calculated by Molinspiration software including molecular polar surface area or molecular volume is available here.

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