

Prediction for a single compound

This option allows you to get data on lipophilicity, solubility and adsorption for a single compound.

To get the prediction

1. enter the name of a compound or its ID
2. Enter pH values
3. Use check boxes logP, Solubility and Absorption to mark characteristics of compound you want to calculate and number of nearest neighbors for these calculations.
4. If you need to know solubility in mg/l or mol/l mark corresponding items.
5. Press OK or Cancel.

Predicted data

Calculate values for pH:

7.4
6.8
5.5

+ Add...(+)
- Delete(-)

Compound ID
benzoic acid

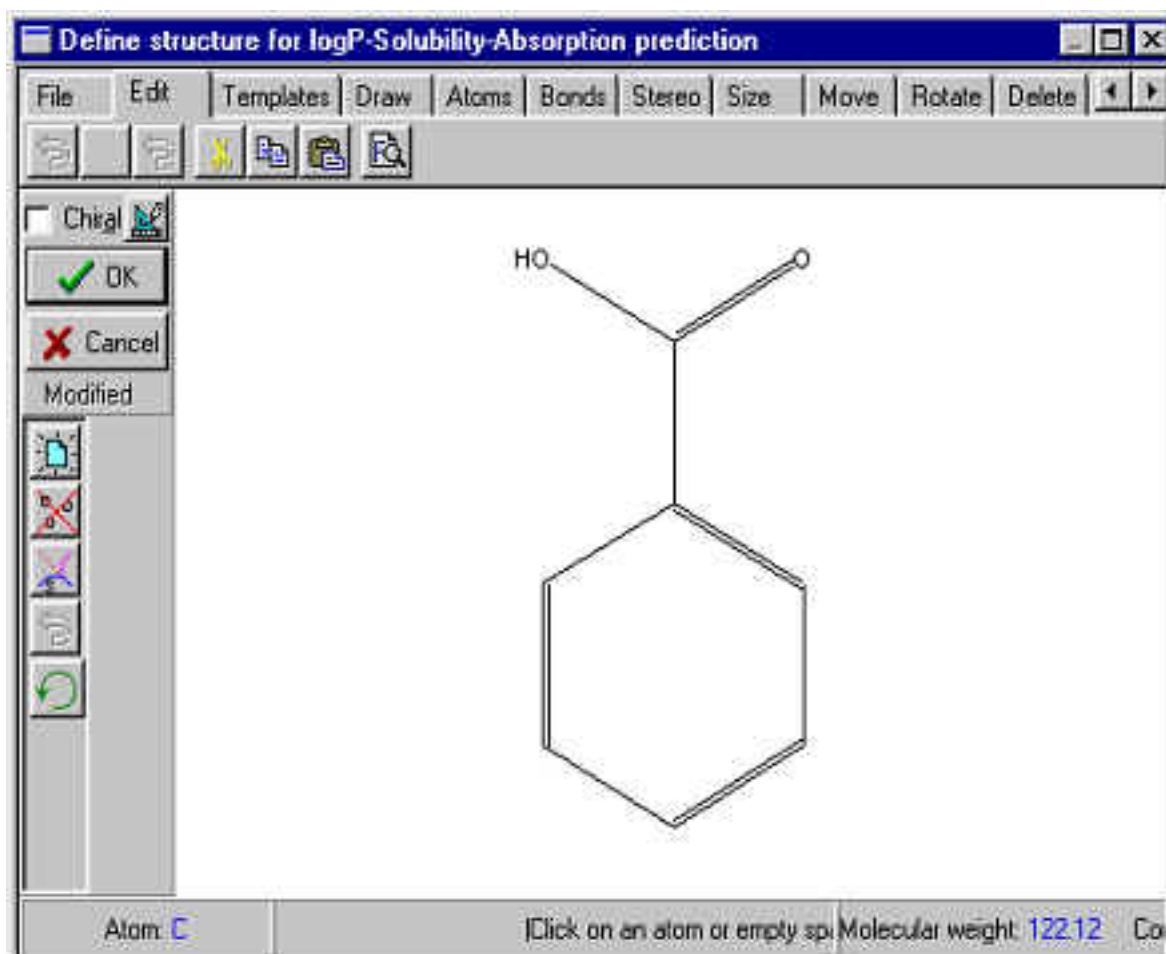
Calculated properties

	No. of neighbours
<input checked="" type="checkbox"/> LogP	5
<input checked="" type="checkbox"/> Solubility	2
<input checked="" type="checkbox"/> Absorption	1

Solubility units

LogSw mol/l g/l

OK Cancel



© The original of this document is available on ScienceDirect.com. For any queries, please contact the corresponding author at shahmoradianpour@shahmoradianpour.com.

