

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

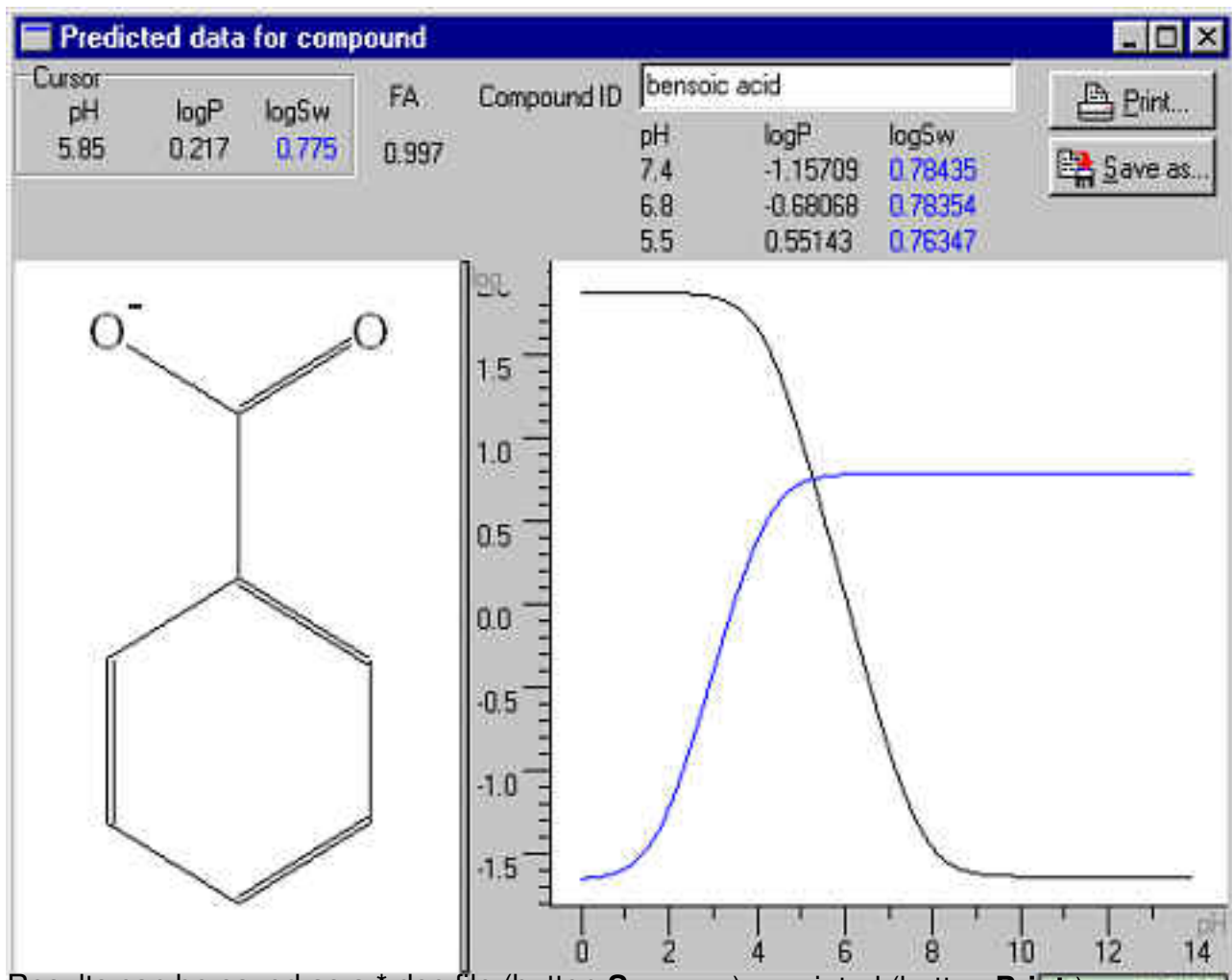
	No. of neighbours
<input checked="" type="checkbox"/> LogP	5
<input checked="" type="checkbox"/> Solubility	2
<input checked="" type="checkbox"/> Absorption	1

Solubility units
 LogSw mol/l g/l

OK Cancel



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