

Using OCHEM predictor

The OCHEM Predictor is a simple one-click prediction tool for OCHEM featured models. Currently the models featured by OCHEM:

- Melting Point (3D descriptors)
- Melting Point (2D descriptors)
- LogP and Solubility
- CYP1A2 inhibition
- Ames test
- Aqueous toxicity (IGC50 for *T. pyriformis*)

You can reach OCHEM Predictor tool by choosing the "Models > Open Predictor" menu item.

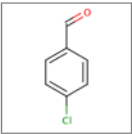
OCHEM Predictor
Predict a number of supported properties/activities for your chemical compounds

What would you like to predict?

- ☐ Melting Point (3D descriptors)
- ☒ Melting Point (2D descriptors)
- ☒ LogP and Solubility
- ☐ CYP1A2 inhibition
- ☐ Ames test
- ☐ Aqueous toxicity (IGC50 for *T. pyriformis*)

[Browse the full list of public models](#)

Select the compounds to be predicted

- ☐ Upload compounds from a file
(SDF/MOL2/SMILES/Excel sheet)
- ☐ Provide a Name/CAS-RN/SMILES
- ☐ Draw Molecule
(click on depiction to the right to draw) 
- ☒ Choose a previously prepared set: [TempLogPow](#)
- ☐ Select molecules by a tag: [\[...\]](#)

☐ Disable prediction cache

First, select the models you would like to apply in the upper part of the Predictor screen. Then, select the molecules you would like to apply the predictions to. You have the choice between:

- Uploading the SDF file with molecule structures
- Providing a Name, CAS-RN or SMILES. The Name and CAS-RN will be used to search for a molecule structure in PubChem
- Drawing a molecule in sketcher
- Selecting a previously prepared dataset (see [Working with datasets](#) for details)
- Selecting all molecules marked by a specific tag

Once you are ready, you can proceed by clicking the "Run predictions!" button. When the prediction process is finished, you are redirected to the predictions browser.

OCHEM predictor - results

Here you can browse the predictions for your compounds and export them in a variety of formats

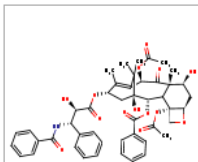
 Export results in a file (Excel, CSV or SDF)

 Add the results as a validation set for model ALogPS 3.0 (updated)

Sorting

1 - 15 of 37

15 items on page 1 of 3 > >>

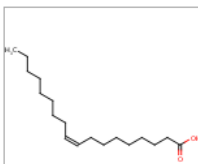


Melting Point (Melting Point - 2D (ALOGPS 2.01 +OESTATE)) = 222.81 °C ± 83.69 (ASNN-STDEV = 37.09, estimated RMSE = 42.70)

logPow (ALogPS 3.0 (updated)) = 3.2 Log unit ± 0.96 (ASNN-STDEV = 0.70, estimated RMSE = 0.49) **CACHED**

logPow(measured) = 0.017

Aqueous Solubility (ALogPS 3.0 (updated)) = 3.65 -log(mol/L) ± 1.60 (ASNN-STDEV = 1.07, estimated RMSE = 0.82) **CACHED**

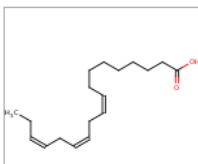


Melting Point (Melting Point - 2D (ALOGPS 2.01 +OESTATE)) = 21.23 °C ± 83.69 (ASNN-STDEV = 20.38, estimated RMSE = 42.70) **CACHED**

logPow (ALogPS 3.0 (updated)) = 7.45 Log unit ± 0.96 (ASNN-STDEV = 0.35, estimated RMSE = 0.49) **CACHED**

logPow(measured) = 3.54

Aqueous Solubility (ALogPS 3.0 (updated)) = 6.87 -log(mol/L) ± 1.60 (ASNN-STDEV = 0.63, estimated RMSE = 0.82) **CACHED**



Melting Point (Melting Point - 2D (ALOGPS 2.01 +OESTATE)) = -28.85 °C ± 83.69 (ASNN-STDEV = 35.30, estimated RMSE = 42.70)

logPow (ALogPS 3.0 (updated)) = 6.58 Log unit ± 0.96 (ASNN-STDEV = 0.68, estimated RMSE = 0.49) **CACHED**

logPow(measured) = 2.51

Aqueous Solubility (ALogPS 3.0 (updated)) = 6.08 -log(mol/L) ± 1.60 (ASNN-STDEV = 1.19, estimated RMSE = 0.82) **CACHED**

You can either review the prediction values in the predictions browser, or export the predictions in the format of your choice (see Exporting data from OCHEM).