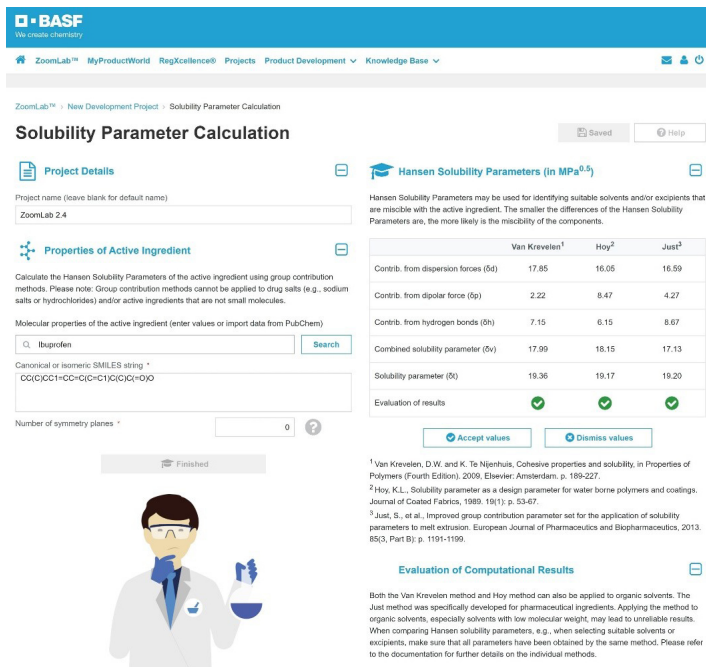


# Calculation of Solubility Parameters is now available in ZoomLab™

Solubility parameters allow rapid screening for suitable excipients such as solvents or polymers that are expected to interact strongly with a given active ingredient. ZoomLab™'s “Solubility Parameter Calculation” module allows for instantaneous calculation of solubility parameters utilizing various group contribution methods described in the pharmaceutical literature!



**Solubility Parameter Calculation**

Project name: ZoomLab 2.4

Properties of Active Ingredient: Bupropfen

SMILES string: CC(C)CC1=CC=CC=C1C1=CC=CC=C1O

	Van Krevelen <sup>1</sup>	Hoy <sup>2</sup>	Just <sup>3</sup>
Contrib: from dispersion forces (Dd)	17.85	16.05	16.59
Contrib: from dipolar force (Dp)	2.22	8.47	4.27
Contrib: from hydrogen bonds (Dh)	7.15	6.15	8.67
Combined solubility parameter (Dv)	17.99	18.15	17.13
Solubility parameter (D)	19.36	19.17	19.20
Evaluation of results	✓	✓	✓

**Evaluation of Computational Results**

Both the Van Krevelen method and Hoy method can also be applied to organic solvents. The Just method was specifically developed for pharmaceutical ingredients. Applying the method to organic solvents, especially solvents with low molecular weight, may lead to unreliable results. When comparing Hansen solubility parameters, e.g. when selecting suitable solvents or excipients, make sure that all parameters have been obtained by the same method. Please refer to the documentation for further details on the individual methods.

ZoomLab™'s “Solubility Parameter Calculation” module calculates Hansen solubility parameters for a user-input compound based on the following group contribution methods:

- Hoftyzer / Van Krevelen
- Hoy
- Just

For calculation, information on the molecular structure of a compound is required in the form of Simplified Molecular Input Line Entry Specification (SMILES). ZoomLab™ then automatically generates the molecular structure, divides the molecule into fragments and assigns the corresponding parameter values for solubility parameter calculation based on the respective group contribution method. The calculated solubility parameters are returned in a result table and information is given whether ZoomLab™ was able to successfully apply the individual group contribution methods.

Find the new “**Solubility Parameter Calculation**” module on **ZoomLab™'s homepage** with the Solubilization modules.

**Register for a Webinar with Pharma Excipients and BASF ZoomLab™: Digitally guiding dosage form and formulation for improved solubility**

Tuesday, June 8th, 2021  
9AM EST | 3PM CET

Register at: <https://lnkd.in/d7ZhGJ6>



## SIGN UP TODAY

Discover for yourself how fast and easy it is to formulate with ZoomLab™ by signing up today – for free! Just enter a few physiochemical properties of the active ingredient and the target dosage form and let ZoomLab™ take care of the rest.

<https://info-mypharma.basf.com/>