

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!

BASF We create chemistry							
A ZoomLab™ MyProductWorld Reg	Knowledge Base 🗸				84		
ZoomLab ^{re} > New Development Project > 8	colubility Parameter Calculation						
Solubility Paramet	er Calculation					🖺 Saved	🕜 Help
Project Details	Hansen Solubility Parameters (in MPa ^{0.5})				1		
Project name (leave blank for default name) ZoomLab 2.4			Hansen Solubility are miscible with Parameters are, t	Parameters may be in the active ingredient. the more likely is the r	used for identifying : The smaller the diffe niscibility of the com	suitable solvents an erences of the Hans sponents.	5/or excipients en Solubility
Properties of Active Ingred	ient	F			Van Krevelen ¹	Hoy ²	Just ³
	Contrib. from dis	spersion forces (õd)	17.85	16.05	16.59		
methods. Please note: Group contribution me salts or hydrochlorides) and/or active ingredie	Contrib. from dip	polar force (õp)	2.22	8.47	4.27		
Molecular properties of the active ingredient (enter values or import data from Pub0	(hem)	Contrib. from hy	drogen bonds (õh)	7.15	6.15	8.67
Q. Ibuprofen		Search	Combined solub	pility parameter (öv)	17.99	18.15	17.13
Canonical or isomeric SMILES string *					10000		
CC(C)CC1=CC=C(C=C1)C(C)C(=0)O			Solubility param	ieter (öt)	19.36	19.17	19.20
			Evaluation of re-	suits	0	0	0
Number of symmetry planes *	0	0		S Accept value	is C) Dismiss values	
(<u>I</u>	Finished		¹ Van Krevelen, D Polymers (Fourth	W. and K. Te Nijenh Edition), 2009, Elsev	uis, Cohesive properier: Amsterdam, p. 1	rties and solubility, in 189-227.	n Properties of
			² Hoy, K.L., Solub	ality parameter as a d	esign parameter for	water borne polyme	rs and coating
19			³ Just, S., et al., Improved group contribution parameter set for the application of solubility parameters to melt extrusion. European Journal of Pharmaceutics and Biopharmaceutics, 20 B5(3, Part B): p. 1191-1199.				
			Evaluation of Computational Results				
			Both the Van Kree	velen method and Ho	y method can also b	e applied to organic	solvents. The

Both the Van Krevelen method and Hay method can also be applied to organic solvents. The Just method was appecially developed for pharmacuciful any predemise, Applying the method to criganic solvents, especially solvents with low molecular weight, may laid to unreliable results. When comparing Hamen solubility parameters, e.g., when setting subble solvents or excepters, make sure that all parameters have been obtained by the same method. Please refer to the documentation for further details on the individual methods.

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TODAY

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

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

and let ZoomLab[™] take care of the rest.

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formulate with ZoomLab[™] by signing up today – for

free! Just enter a few physiochemical properties of the active ingredient and the target dosage form

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