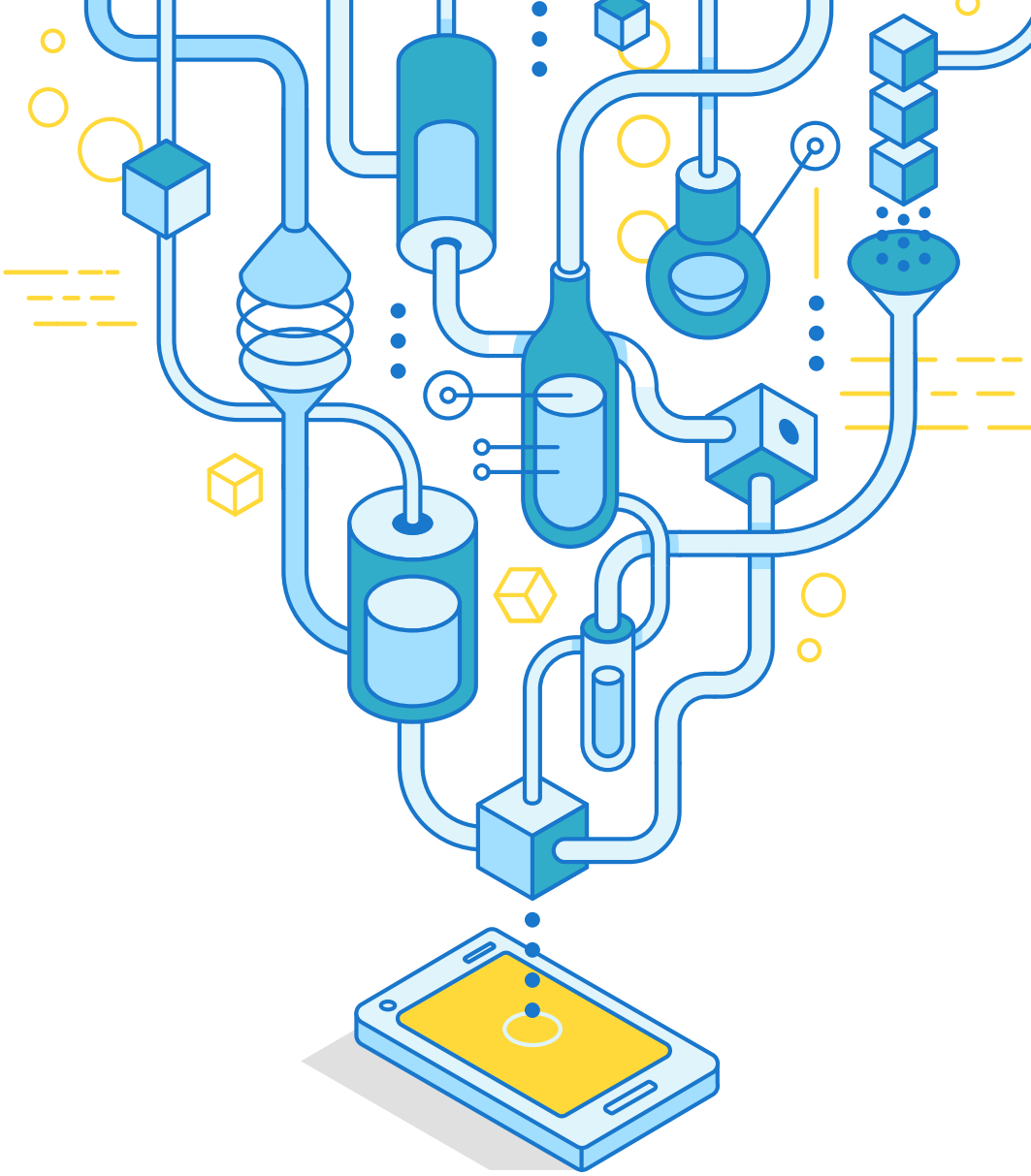
ChemRTP



Real-Time
Chemical Property
Predictor

ChemRTP

www.chemrtp.com

ChemEssen

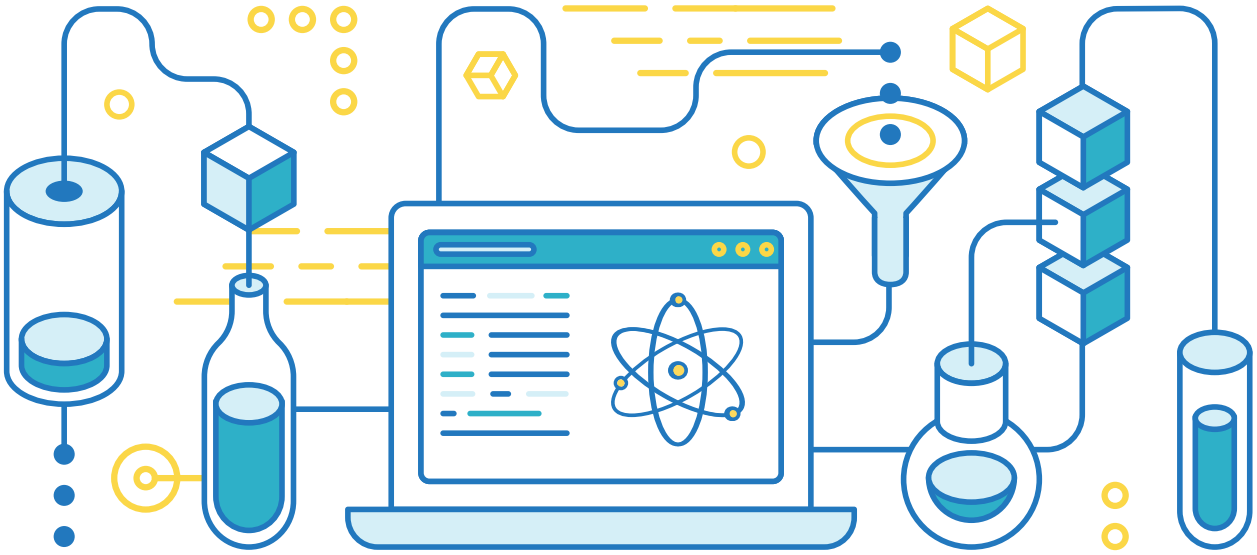
What is **ChemRTP**?

What is Chemical Real-Time Predictor (ChemRTP)?

Chemical Real-Time Predictor (ChemRTP) quickly predicts chemical data and information of chemicals of your interest.

Our versatile QSPR-based ChemRTP provides 28 important chemical data for each chemical in real-time on the web.

Prediction accuracy is also given in cases where experimental data exist.



Type of Properties Provided

	Properties
1	Absolute Entropy of Ideal Gas at 298.15K and 1 bar
2	Acentric Factor
3	Critical Compressibility Factor
4	Critical Pressure
5	Critical Temperature
6	Critical Volume
7	Enthalpy of Formation for Ideal Gas at 298.15 K
8	Liquid Molar Volume at 298.15 K
9	Molecular Weight
10	Net Standard State Enthalpy of Combustion at 298.15 K
11	Normal Boiling Point
12	Melting Point
13	Refractive Index
14	Solubility Parameter at 298.15 K
15	Standard State Absolute Entropy at 298.15 K and 1 bar
16	Standard State Enthalpy of Formation at 298.15 K and 1 bar
17	Magnetic Susceptibility
18	Polarizability
19	Flash Point
20	Parachor
21	Lower Flammability Limit Temperature
22	Lower Flammability Limit Volume Percent
23	Upper Flammability Limit Temperature
24	Upper Flammability Limit Volume Percent
25	Liquid Density at Normal Boiling Point
26	Heat of Vaporization at 298.15 K
27	Heat of Vaporization at Normal Boiling Point
28	Water Solubility

ChemRTP **Information**

Thermo-Physico-Chemical Properties

- Reaction Engineering
- Chemical Process Design / Simulation / Optimization
- Energy Efficiency Improvement for Combustion Processes
- Chemical Safety and Regulation

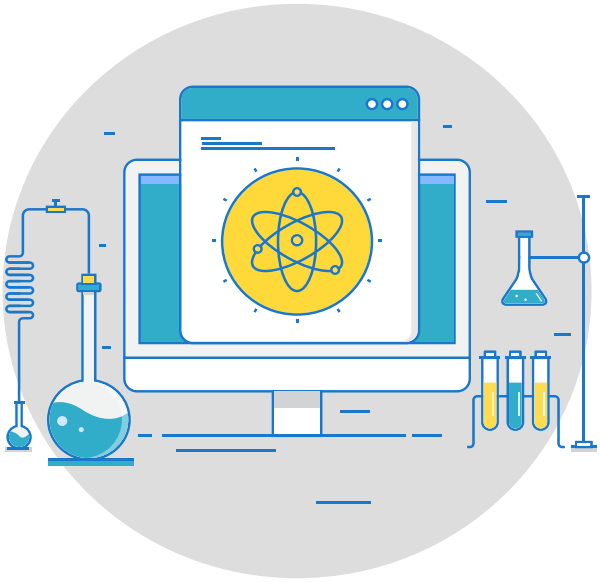
Drug-Related Properties

- New Drug Discovery
- Drug Possibility Provision

ChemRTP **Applications**

- Energy Efficiency Improvement
- Alternative Energy Research
- Environmental Protection
- Process Design, Simulation & Optimization
- Reaction Engineering & Kinetics
- Chemical Process Unit Design & Optimization
- New Drugs Development & Health Researches
- Cosmetics, Flavors & Fragrance Design
- Semiconductor Researches

New Predictor Program



Real-time Chemical Property Prediction.

Able to obtain the property information of chemicals on the real time basis.

Property Values Based on Advanced QSPR.

Able to calculate the property of chemicals including H, C, N, O, S, F, CI, Br, I, P, Si, As based on QSPR Model.

Simple One-Click Tool.

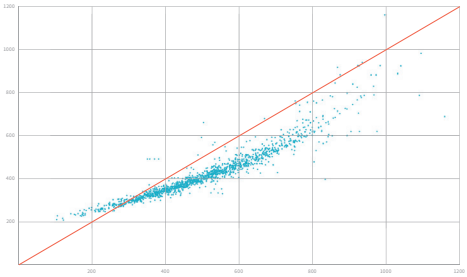
Able to determine a significant number of property data upon entering the chemicals on the website.

Quality Data **Accuracy**

Years of accuracy verification using millions of experimental data points.

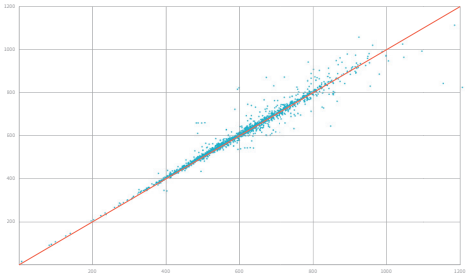
- The experimental data were collected from a broad variety of sources including high impact journals, scientific textbooks, internet, as well as commercial data bases.
- The collected experimental data were inspected and refined to remove the noise and unacceptable errors.
- Refined experimental data were used to verify the accuracy of the estimated values. Thousands of charts were generated and inspected manually on a daily basis.
- A systematic process has now been developed based on chemical analysis theories, e.g., similarity analysis, and was then applied for the accuracy verification

Accuracy of Existing Estimation Methods (Joback Method): **63.07%**



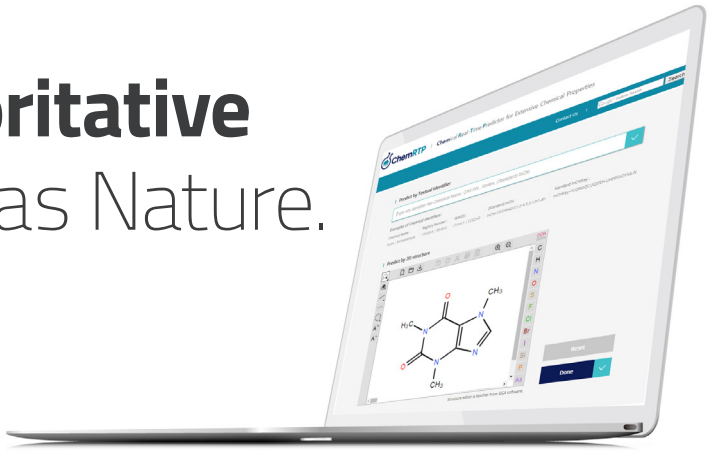
VS

Accuracy of ChemRTP Prediction: **95.02%**



CITATION LIST

Cited in Authoritative Journals such as Nature.



Below is a partial list of collected citations.

PUBLISHER	PUBLICATION
NATURE	Fractal Based Analysis of the Inflence of Odorants on Heart Activity. Hamidreza Namazi, Vladimir V. Kulish. Scientifi Reports 6, Article number: 38555, DOI:10.1038/srep38555 (2016)
NATURE	The Analysis of the Inflence of Odorant's Complexity on Fractal Dynamics of Human Respiration. Hamidreza Namazi, Amin Akrami,Vladimir V. Kulish. Scientifi Reports 6, Article number: 26948, DOI:10.1038/srep26948 (2016)
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American Chemical Society (ACS)	Calculation of Average Molecular Parameters, Functional Groups, and a Surrogate Molecule for Heavy Fuel Oils Using 1H and 13C Nuclear Magnetic Resonance Spectroscopy. Abdul Gani Abdul Jameel, Ayman M. Elbaz, Abdul-Hamid Emwas, William L. Roberts, S. Mani Sarathy. Energy Fuels, 2016, 30 (5), pp 3894–3905, DOI: 10.1021/acs.energyfuels.6b00303 (2016)
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Springer	The CompTox Chemistry Dashboard: a community data resource for environmental chemistry. Antony J. Williams, Christopher M. Grulke, Jeff Edwards, Andrew D. McEachran, Kamel Mansouri, Nancy C. Baker, Grace Patlewicz, Imran Shah, John F. Wambaugh, Richard S. Judson, Ann M. Richard. J Cheminform (2017) 9:61, DOI: 10.1186/s13321-017-0247-6 (2017)
Hindawi	Analysis of the Influence of Complexity and Entropy of Odorant on Fractal Dynamics and Entropy of EEG Signal. Hamidreza Namazi, Amin Akrami, Sina Nazeri, Vladimir V. Kulish. BioMed Research International Volume 2016 Article ID 5469587, 5 pages doi:10.1155/2016/5469587 (2016)
Residue2Heat	THERMO-PHYSICAL CHARACTERIZATION OF FPBO AND PRELIMINARY SURROGATE DEFINITION. Project title: Renewable residential heating with fast pyrolysis bio-oil. A. Frassoldati, A Cuoci, A. Stagni, T. Faravelli, R. Calabria, P. Massoli. Grant Agreement: 654650. Start of the project: 01.01.2016 (48 months)

How To Use ChemRTP

1

Go to www.chemrtp.com.

2

Enter your compound using chemical name or 2D structure.

3

View various property information

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