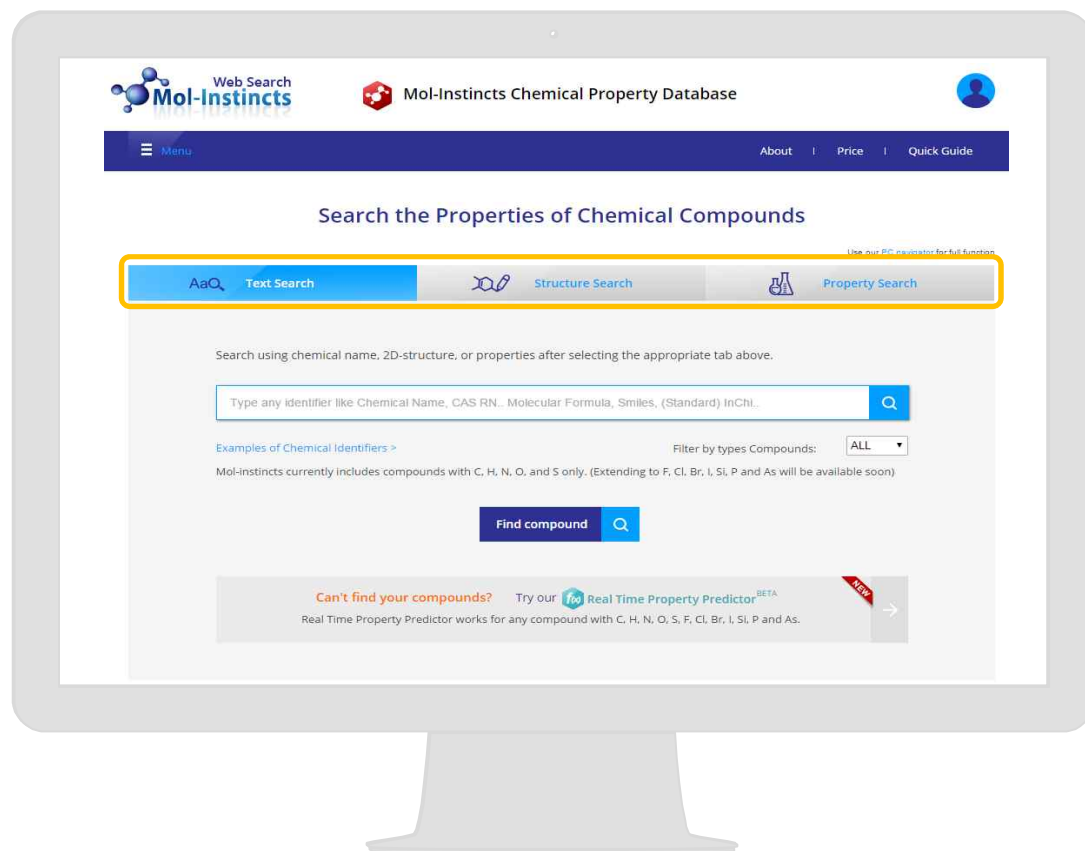




How to Use Mol-Instincts

STEP 1



Select search method

- **Search a compound** : Three searching methods are available

Compound search **TYPE 1**

Search the Properties of Chemical Compounds

Use our [PC navigator](#) for full function

AaQ Text Search Structure Search Property Search


Search using chemical name, 2D-structure, or properties after selecting the appropriate tab above.

benzene

[Examples of Chemical Identifiers >](#) Filter by types Compounds: ALL

Mol-instincts currently includes compounds with C, H, N, O, and S only. (Extending to F, Cl, Br, I, Si, P and As will be available soon)

Find compound

Can't find your compounds? Try our [Real Time Property Predictor](#) ^{BETA}  [→](#)

Real Time Property Predictor works for any compound with C, H, N, O, S, F, Cl, Br, I, Si, P and As.

- **TYPE 1 : Text Search** using textual identification of compound

Compound search **TYPE 2**

Search the Properties of Chemical Compounds

Use our PC navigator for full function

AaQ Text Search Structure Search Property Search

Exact Structure Search
SubStructure Search

Filter by Types of Compounds:
ALL

Reset

Find compound

- **TYPE 2 : Structure Search** using 2D structure of compound

Compound search **TYPE 3**

Search the Properties of Chemical Compounds

Use our PC navigator for full function

AaQ Text Search Structure Search Property Search

	Atom	Minimum	Maximum
Number of Atoms:	C	6	6
	H		
	N		
	O		
	S		

Physical Property: Choose

Min: Max: Unit: Choose Physical Property

Filter by Type of Compound ALL Available to choose type




Reset Find compound

- TYPE 3 : **Property Search** using physical property of compound

STEP 2

Search Result 1000+ compounds found. Click a compound image below to view the data and information. [Quick Guide](#)

1 2 3 4 5 6 7 8 9 10 [>11]

	MOLINSTINCTS ID: 0001-5nm9 Formula: C6H6 IUPAC Name: benzene SMILES: c1ccccc1 InChI: InChI=1/C6H6/c1-2-4-6-5-3-1/h1-6H Matched String: benzene Matching Accuracy: 100.0%	View our data
	MOLINSTINCTS ID: 0001-1gyx Formula: C6H6S IUPAC Name: benzenethiol SMILES: Sc1ccccc1 InChI: InChI=1/C6H6S/c7-6-4-2-1-3-5-6/h1-5,7H Matched String: benzenethiol Matching Accuracy: 86.1%	View our data
	MOLINSTINCTS ID: 0000-4vk9 Formula: C14H22 IUPAC Name: octylbenzene SMILES: CCCCCCc1ccccc1 InChI: InChI=1/C14H22/c1-2-3-4-5-6-8-11-14-12-9-7-10-13-14/h7,9-10,12-13H,2-6,8,11H2,1H3 Matched String: octylbenzene Matching Accuracy: 86.1%	View our data

- Select the compound from the result list

STEP 3

MOLInstincts Web Search

Search another compound by name

MOLINSTINCTS ID: 0001-5nm9
Formula: C6H6
IUPAC Name: benzene
SMILES: c1ccccc1
InChI: InChI=1/C6H6/c1-2-4-6-5-3-1/h1-6H
MIID:0001-5nm9
<http://search.molinstincts.com/properties/constantProperty.ce?0001-5nm9> Cite

Save Data as IKC
Save Descriptor as CSV

Property Data (Constant) | Property Data (Temp. Dependent) | Molecular Descriptor | Quantum Information | Medicine / Drug Information | Spectra Data | Analysis Data

Property	Value	Exp. Data Comparison	Unit
Absolute Entropy of Ideal Gas at 298,15 K and 1 bar			
By Mol-Instincts	64.1857	≤ 1	cal/mol.K
Acentric Factor			
By Mol-Instincts	0.244079	-	-
By Gani	0.206570	-	-
Critical Compressibility Factor			
By Mol-Instincts	0.269630	-	-
By Joback	0.265163	-	-
By Gani	0.263842	-	-
Critical Pressure			
By Mol-Instincts	48.7025	≤ 1%	bar
By Joback	47.6939	≤ 1%	bar
By Gani	47.1919	≤ 1%	bar

Available to save

Available to select

- **View the property data:** 7 different types of compound property information
- **Save data as IKC :** Compatible with other simulation software such as Aspen Plus
- **Save descriptors as CSV :** More than 2,000 descriptors exported to a CSV file by open in MS Excel

Property View **TYPE 1**

Property Data (Constant)	Property Data (Temp. Dependent)	Molecular Descriptor <small>FREE</small>	Quantum Information <small>FREE</small>	Medicine / Drug Information	Spectra Data	Analysis Data
Property		Value	Exp. Data Comparison	Unit		
— Absolute Entropy of Ideal Gas at 298.15 K and 1 bar						
By Mol-Instincts		64.1857	≤ 1	cal/mol.K		
— Acentric Factor						
By Mol-Instincts		0.244079	-	-		
By Gani		0.206570	-	-		
— Critical Compressibility Factor						
By Mol-Instincts		0.269630	-	-		
By Joback		0.265163	-	-		
By Gani		0.263842	-	-		
— Critical Pressure						
By Mol-Instincts		48.7025	≤ 1%	bar		
By Joback		47.6939	≤ 1%	bar		
By Gani		47.1919	≤ 1%	bar		
— Critical Temperature						
By Mol-Instincts		562.5568	≤ 1%	K		
By Joback		570.0280	≤ 1%	K		
By Gani		569.8850	≤ 1%	K		

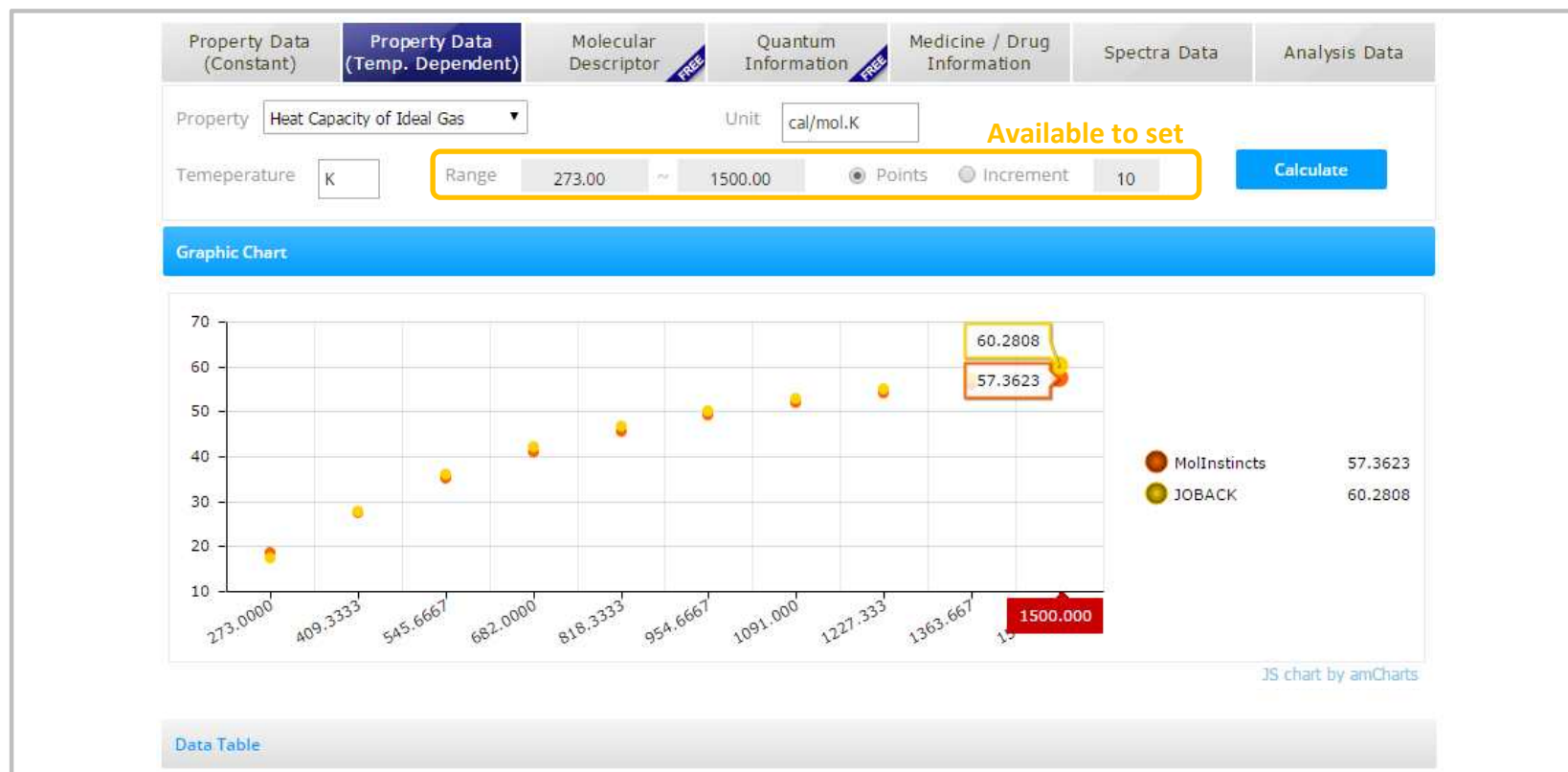
- **TYPE 1 : Thermo-Physical Property - Constant** (35 different categories)
 - Comparison with experimental value
 - Comparison with the existing method as JOBACK, GANI METHOD
 - Prediction value of the compound as Gas/Liquid/Solid

Property View **TYPE 2**

The screenshot displays the 'Property Data (Temp. Dependent)' view in the ChemEssen software. The interface features a navigation bar with tabs for 'Property Data (Constant)', 'Property Data (Temp. Dependent)', 'Molecular Descriptor', 'Quantum Information', 'Medicine / Drug Information', 'Spectra Data', and 'Analysis Data'. Below the navigation bar, there is a 'Property' dropdown menu currently showing a list of 11 thermo-physical properties: 'Please Choose...', 'Heat Capacity of Ideal Gas', 'Heat Capacity of Liquid', 'Heat of Vaporization', 'Liquid Density', 'Surface Tension', 'Thermal Conductivity of Liquid', 'Thermal Conductivity of Gas', 'Vapor Pressure of Liquid', 'Viscosity of Liquid', 'Viscosity of Gas', and 'Second Virial Coefficient'. To the right of the dropdown is a 'Unit' input field. Below these are two radio buttons for 'Points' and 'Increment', and a numerical input field set to '10'. A blue 'Calculate' button is positioned to the right of these controls. At the bottom of the interface, there is a 'Data Table' link and a small text credit 'JS chart by amCharts'.

- **TYPE 2 : Thermo-Physical Property Temperature dependent** (11 different categories)

Property View TYPE 2



- Available to set the number of points or temperature range
- Point value on a graph
- Prediction value pursuant to temperature in data table

Property View **TYPE 3**

Property Data (Constant)		Property Data (Temp. Dependent)		Molecular Descriptor <small>FREE</small>		Quantum Information <small>FREE</small>		Medicine / Drug Information		Spectra Data		Analysis Data	
No	Field	No	Field	No	Descriptor	No	Field	No	Field	No	Field	No	Value
1	Constitutional descriptors	1	Number of atoms	12.0000									
2	Topological descriptors	2	Relative number of C atoms	0.500000									
3	Walk and path counts	3	Relative number of H atoms	0.500000									
4	Connectivity indices	4	Relative number of O atoms	0.00									
5	Information indices	5	Relative number of N atoms	0.00									
6	List of 2D autocorrelation indices	6	Relative number of S atoms	0.00									
7	Edge adjacency indices	7	Number of single bonds	6.0000									
8	Burden eigenvalue descriptors	8	Relative number of single bonds	0.500000									
9	Topological charge indices	9	Relative number of double bonds	0.00									
10	Eigenvalue-based indices	10	Relative number of triple bonds	0.00									
11	Randic molecular profiles	11	Number of aromatic bonds	6.0000									
12	Geometrical descriptors	12	Relative number of aromatic bonds	0.500000									
13	RDF descriptors	13	Relative number of rings	0.083300									
14	3D-MoRSE descriptors	14	Relative number of benzene rings	0.083300									

- **TYPE 3 : Molecular Descriptor** (24 different fields)

Property View **TYPE 4**

Property Data (Constant)	Property Data (Temp. Dependent)	Molecular Descriptor	Quantum Information	Medicine / Drug Information	Spectra Data	Analysis Data
Atoms		12				
Charge		0				
Multiplicity		1				
Electrons		42				
Alpha Electrons		21				
Beta Electrons		21				
Basis Functions		102				
Contracted Shells		36				
Highest Angular Momentum		2				
Largest Deg. of Contraction		6				
Primitive Shells		90				
Vinial Ratio		2.010104064110760E+00				
Total Energy		-2.322486591668341E+02				
Atomic Numbers		6 6 6 6 6				
		1 1 1 1 1				
Nuclear Charges		6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00 6.00000000E+00				
		6.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00 1.00000000E+00				
		1.00000000E+00 1.00000000E+00				
Cartesian Coord.		0.00000000E+00 0.00000000E+00 2.63931183E+00 4.93038066E-32 2.28561299E+00				
		1.31962182E+00 -2.79906863E-16 -2.28561299E+00 1.31962182E+00 1.61607064E-16				
		2.28561299E+00 -1.31962182E+00 3.23222478E-16 0.00000000E+00 -2.63931183E+00				
		-2.79906863E-16 -2.28561299E+00 -1.31962182E+00 0.00000000E+00 0.00000000E+00				
		4.69351366E+00 4.93038066E-32 4.06461540E+00 2.34671737E+00 -4.97771824E-16				
		-4.06461540E+00 2.34671737E+00 2.87389991E-16 4.06461540E+00 -2.34671737E+00				
		5.74789649E-16 0.00000000E+00 -4.69351366E+00 -4.97771824E-16 -4.06461540E+00				
		-2.34671737E+00				
Cartesian Gradient:		0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00				
		0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00 0.00000000E+00				

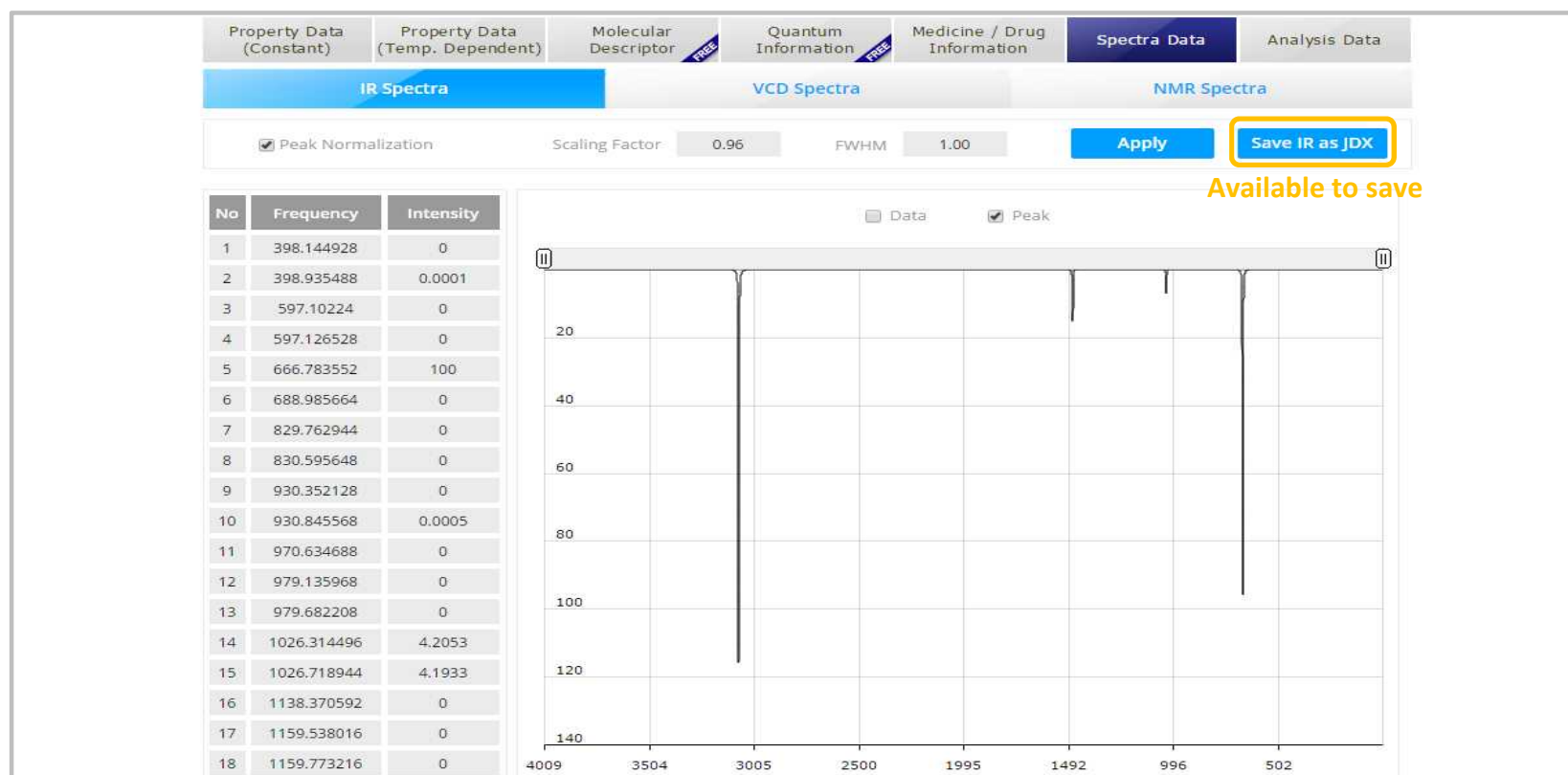
- TYPE 4 : Quantum data

Property View **TYPE 5**

Property Data (Constant)	Property Data (Temp. Dependent)	Molecular Descriptor <small>FREE</small>	Quantum Information <small>FREE</small>	Medicine / Drug Information	Spectra Data	Analysis Data
No	Property Name		Value			
1	Number of atoms		12.0000			
2	molecular weight		78.1118			
3	dipole moment		0.00			
4	LogP (Octanol-Water Partition Coefficient)		2.1520 (≤ 0.1)			
5	LogS (Water Solubility)		-1.6622 (≤ 0.1)			
6	number of acceptor atoms for H-bonds (N,O)		0.00			
7	number of donor atoms for H-bonds (N,O)		0.00			
8	Ghose-Crippen molar refractivity		26.0580			
9	Ghose-Crippen octanol-water partition coeff. (logP)		1.8300			
10	Moriguchi octanol-water partition coeff. (logP)		2.2550			
11	Lipinski Alert index		0.00			
12	Drug-likeness		non-drug			
13	Activity Score for GPCR ligands		-3.6930			
14	Activity Score for Ion Channel Modulators		-3.6410			
15	Activity Score for Kinase Inhibitors		-3.8030			
16	Activity Score for Nuclear receptor ligands		-3.9990			

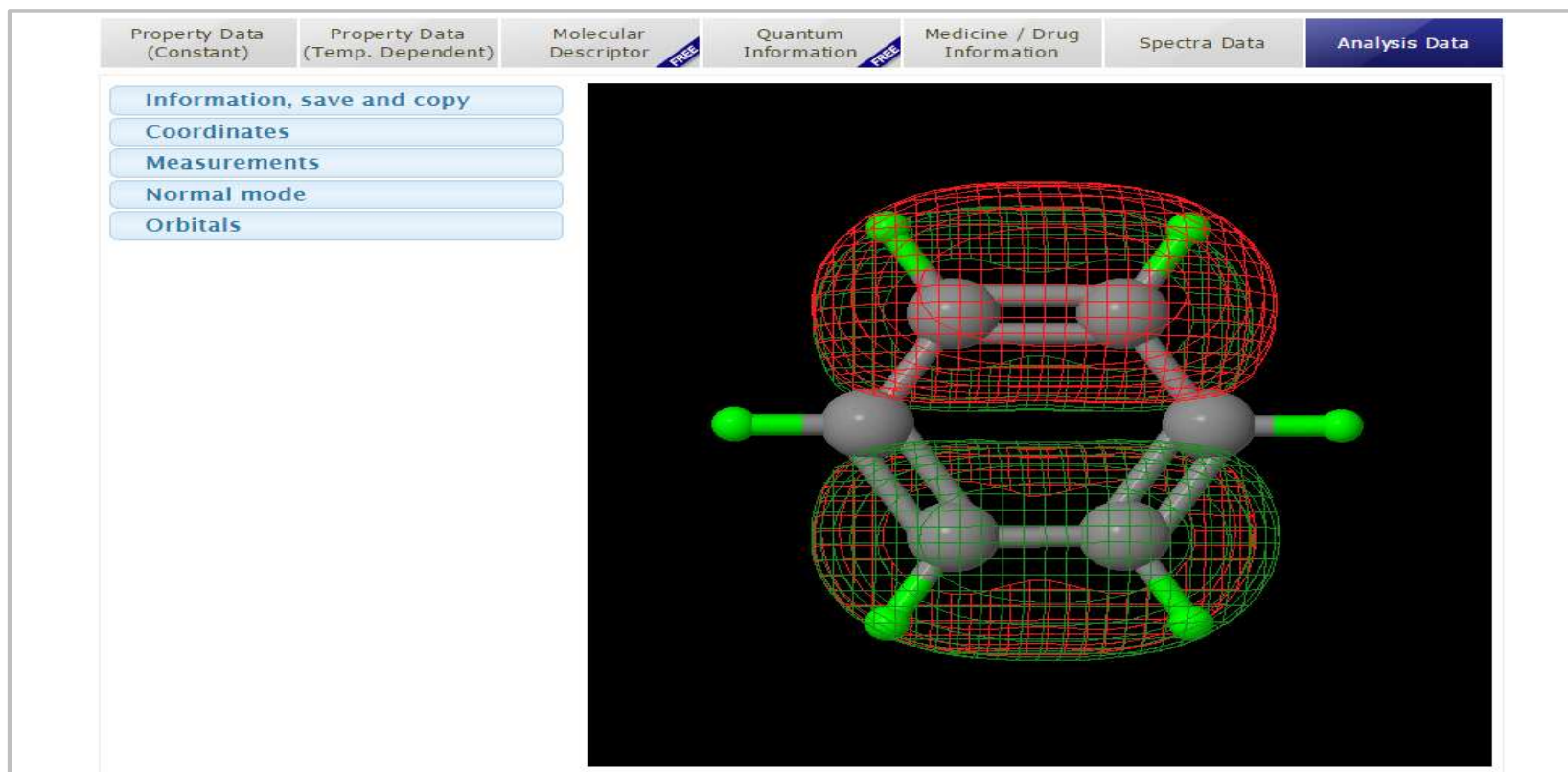
- **TYPE 5 : Drug-Related Property** (16 different data)

Property View **TYPE 6**



- **TYPE 6 : IR / VCD / NMR spectra data**
 - Available to save IR data as JDX file accessible by open in MS Excel, Word, or Notepad

Property View **TYPE 7**



The screenshot displays a software interface with a top navigation bar containing several tabs: "Property Data (Constant)", "Property Data (Temp. Dependent)", "Molecular Descriptor", "Quantum Information", "Medicine / Drug Information", "Spectra Data", and "Analysis Data". The "Analysis Data" tab is currently selected and highlighted in blue. Below the navigation bar, on the left side, there is a vertical list of menu items: "Information, save and copy", "Coordinates", "Measurements", "Normal mode", and "Orbitals". The "Orbitals" item is selected, and its content is displayed in a large central window. This window shows a 3D ball-and-stick model of a molecule with two large, red, wireframe mesh surfaces representing molecular orbitals. The atoms are colored in shades of gray and green. The background of the central window is black.

- **TYPE 7 : Molecular Orbital Information**