

Molecular Modeling Pro™

This advanced molecular modeling program is the result of over 20 years of development at a major chemical company. Developed first for main-frame computers, it now is available for Windows. Molecular Modeling Pro has most of the advanced features available in expensive PC-based molecular modeling programs and more! It probably has the most physical property calculations from structure of any program sold for the PC.

Molecules are easily constructed with your mouse and pull-down menus. The program can display molecules as wire frame, ball and stick, spheres and dot surface models. Up to 5000 atoms and 40 molecules can be displayed on the screen at a time and minimized using the MOLY minimizer. In addition, for those with WIN 95/98 or WIN NT an MM2 minimizer and minimization with MOPAC 6.0 is also included. The AMBER minimizer in Chemsite Pro also accessible from within MMP (requires Chemsite Pro). Routines for conformational analysis are also included.

The Molecular Modeling Pro program is:

- a physical property estimation program
- a 3-D chemical structure drawing program
- a chemical data base creation program (used with the companion Molecular Analysis Pro program)
- a molecular graphics modeling tool
- a reaction/mixture editor
- a computer slide show maker
- a batch structure printing program
- an unsophisticated structural/reaction searching program
- a program capable of converting connection table formats between MOLfiles and MACROMODEL files

Calculations made by Molecular Modeling Pro

Mass, size

- Molecular weight
- Van der Waals volume (calculated with geometry)
- Molar volume (van Krevelen type method)
- Surface area (calculated with geometry)
- Length, width, depth (current, maximum and minimum calculated by geometry)
- Density (proprietary method for small molecules)
- Mass Percent

Partition coefficients, hydrophobicity, solubility etc.

- Log water octanol partition coefficient (4 methods, Fragment addition generally following the methods of Hansch and Leo, atom based generally following Ghose and Crippen, charge and atom based, and Q Log P after N. Bodor and P. Buchwald, J. Phys. Chem. B, 1997, 101: 3404-3412)
- HLB (hydrophilic lipophilic balance, proprietary method)
- Hydrophilic surface area (proprietary method)
- Percent hydrophilic surface area (proprietary method)
- Polar surface area (J. Med. Chem. 43: 3714-3717)
- Hydration number
- Water solubility (after Klopman et.al. J. Chem. Inf. Comput. Sci. 32:474 and S. Yalkowsky, J. Pharm Sci., 70:971)
- Olive oil gas partition coefficient (after Klopman et.al. J. Med. Chem. 43: 3714-3717)

Properties used in QSAR

- Sterimol properties (L1, B1, B2, B3, B4, B5 and 3 more)
- Hammett Sigma (sigma para, meta, sigma induction (SIND), sigma star)(proprietary method)

- MR (molar refractivity after Ghose and Crippen)

Dipole moment and other charge related properties

- Dipole moment (Modified methods based on Del Re method: G. Del Re, J. Chem. Soc. 4031 (1958); D. Poland and H.A. Scheraga, Biochemistry 6: 3791 (1967); Coefficients modified in MAP 4.0 to take into account pi contributions ; PEOE method: J. Gasteiger and M. Marsili, Tetrahedron 36:3219 (1980); MPEOE (DQP) method: K.T. No, J.A. Grant and H.A. Scheraga, J. Phys. Chem. 94:4732 (1990) and K.T. No, J.A. Grant, M.S. Jhou and H.A. Scheraga, J. Phys. Chem. 94: 4740 (1990); J.M. Park, K.T. No, M.S. Jhou and H.A. Scheraga, J. Comp. Chem. 14:1482 (1993). Semi-empirical Quantum Mechanics methods in CNDO and MOPAC are alternative methods used by MMP to calculate dipole moment.
- Partial charge (many methods - see Dipole moment)
- HOMO/LUMO (via CNDO or MOPAC)
- Hydrogen bond acceptor and donor from charge calculations

Connectivity indices

- Randic, Hall, Kier type connectivity indices 0-4
- Randic, Hall, Kier type valence indices 0-4
- Kier type Kappa shape index 2
- Wiener index
- Chemically Intuitive Molecular Index (F. Burden, Quant. Struct.-Act.Relat. 16:309-314 (1997))

Thermodynamics

- Critical temperature, pressure and volume (after Joback and Reid)
- Normal boiling and freezing point (after Joback and Reid)
- Enthalpy of formation, ideal gas at 298 K (after Joback and Reid)
- Gibbs energy of formation, ideal gas, unit fugacity at 298 K
- Enthalpy of vaporization at the boiling point (after Joback and Reid)
- Enthalpy of vaporization at the boiling point (after Joback and Reid)
- Enthalpy of fusion (after Joback and Reid)
- Liquid viscosity (after Joback and Reid)
- Heat capacity, ideal gas (after Joback and Reid)
- Effective number of torsional bonds (tau) (after S. Yalkowsky et.al.)
- Hydrogen Bond Number (after S. Yalkowsky et.al.)
- Entropy of boiling (after S. Yalkowsky et.al.)
- Effective number of torsional bonds (tau) (after S. Yalkowsky et.al.)
- Heat capacity change on boiling (after S. Yalkowsky et.al.)
- Vapor pressure (after S. Yalkowsky et.al.)
- Vapor pressure (after The Handbook of Chemical Property Estimation Methods)
- Boiling point (after The Handbook of Chemical Property Estimation Methods)
- Parachor (after The Handbook of Chemical Property Estimation Methods)

More properties are available through the MOPAC program included., such as heat of formation, ionization potential and many more.

Polymer and Surfactant properties

- Solubility parameter
- 3-D solubility parameters (dispersion, polarity and hydrogen bonding)
- Water content of polymers at different relative humidities
- Melt transition temperature
- Glass transition temperature
- Chain length (van Krevelen Z)
- Surface tension of liquids
- Surface tension in water
- Molecular weight, molar volume, van der Waals volume, surface area (listed above)

- HLB, hydrophilic surface area, % hydrophilic surface area (listed above)

Text

- Molecular formula
- SMILES notation

