

Definitions of properties with experimental or predicted values in REGISTRY

Property name	Definition	Experimental Values Available	Predicted Values Available
Bioconcentration Factor	Ratio of the concentration of a substance in an aquatic organism to the average concentration of the substance in the surrounding water.		√
Boiling Point	Temperature (Degrees Celsius) at which the vapor pressure of a liquid is equal to the pressure of the atmosphere.	√	√
Density	Mass per unit volume of a substance expressed in grams per cubic centimeter as the default units.	√	√
Electrical Conductance	An indication of the ease with which electric current flows through a material as defined by the ratio of current carried through the material to the difference in the potential applied.	√	
Electrical Conductivity	Electric conductance per unit of area or volume.	√	
Electrical Resistance	An indication of how strongly a material opposes the flow of electric current as defined by the ratio of the voltage applied to the electric current that flows through it.	√	
Electrical Resistivity	Electric resistance per unit of area or volume.	√	
Enthalpy of Vaporization	Amount of energy (kJ/mol) needed to convert a liquid to vapor at its boiling point.		√
Flash point	Minimum temperature (Degrees Celsius) at which a liquid or volatile solid gives off sufficient vapor to form an ignitable mixture with air.		√
Freely Rotatable Bonds	Total number of single, non-ring bonds about which rotation causes a significant physiochemical change in the relative position of the atoms in a molecule.		√

Property name	Definition	Experimental Values Available	Predicted Values Available
Glass Transition Temperature	Approximate midpoint in the temperature range over which an amorphous material transitions from a hard, glassy, or brittle condition to a flexible fluid or elastomeric condition.	√	
Hydrogen Acceptors	Sum of the number of Nitrogen and Oxygen atoms in the molecule (These atoms are capable of forming hydrogen bonds with the Hydrogen atoms attached to Nitrogen or Oxygen atoms).		√
Hydrogen Donors	Total number of Hydrogen atoms attached to the Nitrogen and/or Oxygen atoms in the molecule (These Hydrogen atoms are capable of forming hydrogen bonds with hydrogen acceptor atoms)		√
Intrinsic Solubility (molar)	The solubility of the neutral form of a compound expressed in moles of solute per liter of solution.		√
Intrinsic Solubility (mass)	The solubility of the neutral form of a compound expressed in grams of solute per liter of solution.		√
Koc - (Organic Carbon Adsorption Coefficient)	For a substance added to a mixture of soil and water, Koc is the ratio of the amount of the substance adsorbed per unit weight of organic carbon in the soil to the concentration of the substance remaining in the water at equilibrium.		√
logP	Logarithm of the partition coefficient between octanol and water for the neutral form of a compound		√
logD	Logarithm of the partition coefficient between octanol and water at a given pH for the mixture of the neutral and ionic forms of a compound		√

Property name	Definition	Experimental Values Available	Predicted Values Available
Magnetic Moment	Ratio of torque exerted on an atom or molecule by a magnetic field to the field strength.	√	
Mass Solubility	The number of grams of a compound that dissolve in pure water at 25 °C to produce a liter of saturated solution.		√
Median Lethal Dose	Statistical estimate of the dose for a given substance that would cause death in 50% of test subjects. The organism and route of administration are also included when reported.	√	
Melting Point	Temperature at which a substance changes from the solid to the liquid state. A solvent listed with a melting point indicates the solvent from which the substance was recrystallized.	√	
Molecular Weight	Sum of the atomic weights of the atoms in a molecule calculated using the 1997 IUPAC atomic weights		√
Molar solubility	Number of moles of a compound that dissolve in pure water at 25 degrees C to produce a liter of saturated solution		√
Molar Volume	The volume per quantity of a substance expressed in cubic centimeters per mole.		√
Optical Rotatory Power	Degree of rotation to the left (-) or right (+) of the plane of polarization of a beam of light upon passing through a molecule containing one or more asymmetric carbon atoms.	√	

Property name	Definition	Experimental Values Available	Predicted Values Available
pKa	Negative logarithm of the acid-base dissociation constant (in the range of 0 to 14) at 25 degrees C and zero ionic strength in aqueous solutions for the most acidic and/or most basic sites in a molecule. The pKa for the most basic site is the pKa of the molecule after the most basic site has been protonated.		√
Polar Surface Area	The sum of the surface areas of polar atoms (oxygen, nitrogens, and attached hydrogens) in a molecule expressed in Angstroms squared.		√
Refractive Index	Ratio of the sine of the angle of incidence to the sine of the angle of refraction for a light ray passing through the interface of two media.	√	
Tensile Strength	Maximum longitudinal stress a material subjected to a stretching load can withstand without tearing.	√	
Vapor pressure	Pressure exerted by a vapor in equilibrium with its liquid or solid form at 25 C.		√

Experimental Spectra Types in REGISTRY

¹H-NMR
¹³C-NMR
¹⁹F-NMR
³¹P-NMR
²⁹Si-NMR
 IR
 Raman
 Mass Spec