administering the active pharmaceutical ingredient (API) for purposes of assessing safety in preclinical models, early- to late-phase human clinical trials, and for routine clinical/commercial use. This overview discusses approaches for creating small-molecule API dosage forms, from preformulation to commercial manufacturing.

Yalkowsky, S. H. and D. Alantary (2018). "Estimation of melting points of organics." *J Pharm Sci* 107(5):1211–1227.

Unified physicochemical property estimation relationship is a system of empirical and theoretical relationships that relate 20 physicochemical properties of organic molecules to each other and to chemical structure. Melting point is a key parameter in the unified physicochemical property estimation relationships scheme because it is a determinant of several other properties including vapor pressure, and solubility. This review describes the first-principals calculation of the melting points of organic compounds from structure. The calculation is based on the fact that the melting point, Tm, is equal to the ratio of the heat of melting, DeltaHm, to the entropy of melting, DeltaSm. The heat of melting is shown to be an additive constitutive property. However, the entropy of melting is not entirely group additive. It is primarily dependent on molecular geometry, including parameters which reflect the degree of restriction of molecular motion in the crystal to that of the liquid. Symmetry, eccentricity, chirality, flexibility, and hydrogen bonding, each affect molecular freedom in different ways and thus make different contributions to the total entropy of fusion. The relationships of these entropy determining parameters to chemical structure are used to develop a reasonably accurate means of predicting the melting points over 2000 compounds.

Partitioning

Al-Badr, A. A. and G. A. Mostafa (2014). "Pravastatin sodium." *Profiles Drug Subst Excip Relat Methodol* 39:433–513.

Pravastatin sodium is an [HMG-CoA] reductase inhibitor and is a lipid-regulating drug. This monograph includes the description of the drug: nomenclature, formulae, elemental composition, solubility, appearance, and partition coefficient. The uses and the methods that have been reported for the synthesis of this drug are described. The physical methods that were used to characterize the drug are the X-ray powder diffraction pattern, thermal methods, melting point, and differential scanning calorimetry. This chapter also contains the following spectra of the drug: the UV spectrum, the vibrational spectrum, the nuclear magnetic resonance spectra, and the mass spectrum. The compendial methods of analysis include the British Pharmacopoeia and the United States Pharmacopoeia methods. Other methods of analysis that are included in this profile are spectrophotometric, electrochemical, polarographic, voltammetric and chromatographic, and immunoassay methods. The chapter also contains the pharmacokinetics, metabolism, stability, and articles that reviewed pravastatin sodium manufacturing, characterization, and analysis. One hundred and sixty-two references are listed at the end of this comprehensive profile.

Andres, A. et al. (2015). "Setup and validation of shake-flask procedures for the determination of partition coefficients (logD) from low drug amounts." *Eur J Pharm Sci* 76:181–191.

Several procedures based on the shake-flask method and designed to require a minimum amount of drug for octanol–water partition coefficient determination have been