UPPER: Unified Physical Property Estimation Relationships

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As the synthesis of new compounds becomes more efficient, the importance of estimating environmentally, pharmaceutically, and industrially relevant physical properties of molecules becomes more valuable. Experimental determination is expensive and time consuming and thus is seldom justified at an early development stage. A semi-empirical model has been developed to provide a simple means of estimating physical properties of wide range of environmentally and pharmaceutically relevant organic compound including: enthalpy, entropy, heat capacity, vapor pressure, solubility, partition coefficient, melting point, boiling point, air-octanol partition coefficient, molar volume, activity coefficient, and air-water partition coefficient.

Experimental values of the heat capacity, enthalpy, heat capacity, aqueous solubility, partition coefficient, melting point, of over 400 hydrocarbons were collected from the literature and also from MPBPVP™ 3.2 EPA, Kowwin™ 3.2EPA and the AQUASOL database. 20 different physical properties were calculated using the group contribution method and non additive molecular descriptors like symmetry and flexibility. The group contribution values for calculating the predicted enthalpy of melting and boiling, molar volume and activity coefficient were generated using multiple linear regression models using SPSS (version10.0). All other analysis was performed using Microsoft Excel 2003.

The results are summarized in Table I.

This model is simple to use, accurate and applicable to wide variety of organic compounds.

Table I: Summary of UPPER estimation results.

Physical Property	Number of compounds	Range of exp. data low	Range of exp. data high	Average abs. error	Units
Heat of Boiling	395	9.7	57.2	0.74	kJ/mol
Entropy of Boiling	379	68.6	103.8	3.1	J/K mol
Heat Capacity of Boiling	332	-132	-56	8.9	J/K mol
Boiling Point	394	112	627	6.2	K
Heat of Fusion	37	2.3	12.6	2.2	kJ/mol
Entropy of Fusion	63	8.5	139.7	9.5	J/K mol
Melting Point	256	85	374	28.1	K
Molar Volume	255	34.4	352.8	2.18	cc/mol
log (Vapor Pressure)	246	-7.85	1.87	0.19	log (atm)
log Koa	190	-3.2	5.6	0.17	L/(atm mol)
log Sw	65	-7.32	-1.05	0.56	mol/L
log Kow	99	0.37	8.31	0.32	unitless