Exploring Physical Properties and Thermodynamic Relationships with the Help of the Dortmund Data Bank (DDB) and DDB Software Package (DDBSP)

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Since 2001 a special educational version of the Dortmund Data Bank is available as single PC or classroom license containing the greater part of the software plus approx. 33 000 data sets for 30 common components.

This package allows the student to easily explore a large variety of phenomena in pure component and mixture behavior and to gain experience with the applicability and reliability of a broad range of estimation methods (Joback, Benson, UNIFAC, mod. UNIFAC, PSRK, …).

The package is especially valuable to:

- incorporate modern methods and data into teaching
- have the students examine real world experimental data
- let them get acquainted to experimental scattering and reliability of data
- get hands on experience with a large variety of estimation method
- teach them to use the sophisticated tools for physical property estimation, which are also used by many companies worldwide
- let them explore thermodynamic relationships between different types of data (e.g. pure component vapor pressures and enthalpy of vaporization, ….)
- let them explore the performance of thermodynamic models for the simultaneous description of different types of data (VLE, h^E,…)

Several examples are given below

Experimental Pure Component and Mixture Data Available in the Educational Version of DDB/DDBSP

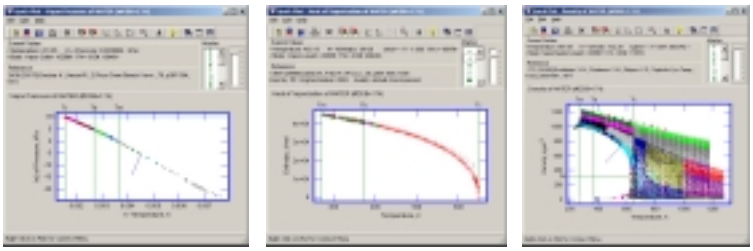
	data sets	data points	references
Critical Data	469	469	268
Vapor Pressure	3703	18658	2226
Enthalpy of Vaporization	398	1634	200
Melting Point	744	843	450
Enthalpy of Fusion	124	125	87
Density	5744	40197	1800
2. Virial Coefficient	208	949	121
Ideal Gas Heat Capacity	145	2065	100
Molar Heat Capacity	1854	13145	330
Entropy	136	224	96
Dielectric Constant	13	109	7
Viscosity	3771	19250	1033
Kinematic Viscosity	355	1090	86
Surface Tension	526	2395	206
Thermal Conductivity	1852	14994	385
...	...	...	...
sum	**20369**	**118524**	

Phase Equilibria			
Vapor-Liquid Equilibria	normal boiling substances	2942	data sets
Vapor-Liquid Equilibria	low boiling substances	1898	data sets
Vapor-Liquid Equilibria	electrolyte systems	206	data sets
Liquid-Liquid Equilibria		1587	data sets
Activity Coefficients	infinite dilution (in pure solvents)	2066	data points
Activity Coefficients	infinite dilution (in mixtures)	94	data sets
Gas Solubilities		1111	data sets
Solid-Liquid Equilibria	mainly organic compounds	368	data sets
Salt solubilities	mainly in water	176	data sets
Azeotropic Data		4333	data points

Excess Properties			
Excess Enthalpies		2095	data sets
Excess Heat Capacities		137	data sets
Excess Volumes		1572	data sets

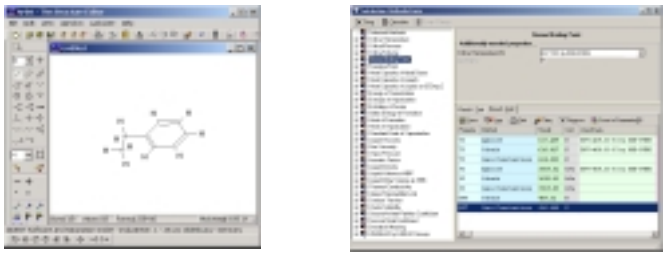
Experimental Pure Component Properties (PURE)

More than 20000 data sets (nearly 120000 data points) from literature can easily be retrieved from the PURE data bank. Different graphical representations give a deep insight into the thermophysical behavior of the different components over a large temperature and pressure range. Data are easily exportable to allow for any further processing in spreadsheet or user programs. Thermodynamic relationships like the Clausius-Clapeyron equation can e.g. be examined using liquid and solid vapor pressures over a large temperature range, heat of fusion and heat of vaporization data and liquid and vapor densities.



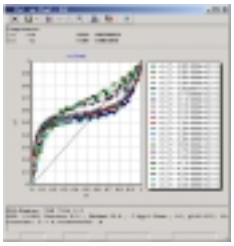
Estimation of Pure Component Properties (ARTIST)

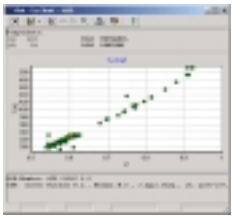
The knowledge of different pure component properties is of great importance for solving problems in the design and optimization of chemical processes, environmental protection, risk assessment, …A student should be familiar with the different approaches to property estimation, especially the commonly used group contribution methods. To simplify property estimation, the program ARTIST automatically estimates a variety of properties using different methods. The molecular structure can be drawn by the user or loaded from the structure data base.



Experimental Data for Mixtures (MIX)

The real behavior of liquid mixtures is of great importance for many practical applications. With the help of a very large number of experimental phase equilibrium and excess property data for binary and higher mixtures the student is able to explore a variety of phenomena including the occurrence of azeotropic behavior and its variation with temperature, liquid-liquid equilibria, gas solubilities, … Phase equilibrium data and osmotic coefficients for electrolyte systems are included to demonstrate the effect of ionic species on the solvent fugacity (salting in and salting out). A variety of graphical representations, data correlation (g^E-models and equations of state) and prediction (UNIFAC, mod. UNIFAC, PSRK, …) help the student to become familiar with different aspects of mixture thermodynamics including modeling and estimation.





Simultaneous Regression of Mixture Data (Recval/3)

Recval/3 was developed for the simultaneous regression of vapor-liquid equilibria, azeotropic data, activity coefficients at infinite dilution, liquid-liquid equilibria, solid-liquid equilibria, excess enthalpies and excess heat capacities with the help of different g^E-models. This enables the student to gain more understanding for the interdependence of the different types of mixture data. The student will learn to judge the reliability and quality of the experimental data from literature by comparing the data from different authors, checking the consistency of VLE data with the help of established thermodynamic tests and examine e.g. the temperature dependence of VLE, azeotropic or γ^∞ data with excess enthalpy and excess heat capacity data.

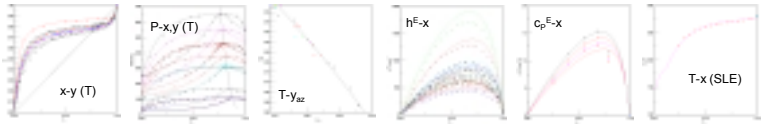


Figure: Different Data for the System Cyclohexane (1) – 1-Propanol (2) together with curves from the Wilson equation (temperature dependent interaction parameters)