**Structural Property Relation**

|  |  |  |
| --- | --- | --- |
| **No.** |  | **Source/Remarks** |
| **LIQUID HEAT CAPACITY** | | |
| 1 |  | Maranas 1996 |
| 2 | We may conclude that Cs p, and Cl p are additive molar functions; their group contributions, also valid for polymers, are given in Table 5.1.    if experimental data are lacking, the temperature function of the heat capacity may be approximated with these average values, so that, with T in K:    With the aid of Eqs. (5.7) and (5.8) the specific heat capacity in the solid and the liquid state at temperatures of practical interest may be predicted approximately from their values at room temperature.  Wunderlich et al. (1988) have confirmed the linear temperature dependence of the liquid heat capacities and derived group contributions for the whole temperature range of 250–750 K. His values are reproduced in Table 5.4 | Properties of Polymers  <https://www.unpa.edu.mx/~aramirez/propiedades%20de%20polimeros.pdf>  Pg. 110-111  Pg. 115-116 |
| 3 | 6.19-6.24 Ruzicka & Domalski (Got T dependence) |  |
| **VAPOUR PRESSURE** | | |
| 1 | Whenever a few reliable vapor-pressure data are at hand, they should be used for cautious interpolation and extrapolation. The correlation given here is to be used only when no reliable vapor-pressure data at all are available.  The AMP Equation Extending a suggestion by Moelwyn-Hughes (1961), Abrams et al. (1974) presented an equation relating pressure P to absolute temperature T:    Here Vw is the (hard-core) van der Waals volume; E0 is the enthalpy of vaporization of the hypothetical liquid at T = 0; s is the number of equivalent oscillators per molecule and R is the gas constant (82.06 cm3-atm/g-mol K); E0/R is in kelvins and the universal constant a is equal to 0.0966 when P is in atm and T is in kelvins. Abrams et al. (1974) and Macknick et al. (1977) have shown that this equation gives reliable results for large molecules and that it is suitable for representing vaporpressure data in the range 10-6 to 2 atm. | Vapor Pressures of Heavy Liquid Hydrocarbons by a Group-Contribution Method  <https://pubs.acs.org/doi/pdf/10.1021/i160072a010>  Vapor Pressures of Liquids as a Function of Temperature. Two-Parameter Equation Based on Kinetic Theory of Fluids  <https://pubs.acs.org/doi/pdf/10.1021/i160051a018>  <https://pubs.acs.org/doi/pdf/10.1021/i160063a019> (corrections) |
| 2 | See Pg. 108-112 for group contributions | Group-contribution method for the estimation of vapor pressures  <https://www.sciencedirect.com/science/article/pii/0378381294800251> |
| 3 | where ai is the regression coefficient for the ith fragment, fi is the number of times the ith fragment occurs in the structure, n is the number of cases, s is the standard error of the regression, r2 is the explained variance, and F is the appropriate f-test statistic  see Pg. 1712 – 1713 for group contributions | A Simple Structure-Based Calculator for Estimating Vapor Pressure  <https://pubs.acs.org/doi/pdf/10.1021/jf980922%2B> |
| 4 | Contains a lot of literature | QUANTITATIVE STRUCTURE–PROPERTY RELATIONSHIPS FOR PREDICTION OF BOILING POINT, VAPOR PRESSURE, AND MELTING POINT  <https://setac.onlinelibrary.wiley.com/doi/pdf/10.1897/01-363> |
| **HEAT OF VAPORISATION** | | |
| 1 |  | <https://www.sciencedirect.com/science/article/pii/S0378381218302425>  references joback |
| 2 |  | <https://www.sciencedirect.com/science/article/pii/S0378381218302425>  very complicated method |
| 3 | See Pg. 168 – 169, 170 for group contributions | Estimation of the enthalpy of vaporization at normal boiling temperature of organic compounds by a new group contribution method  <https://www.sciencedirect.com/science/article/pii/S0378381218302425> |
| 4 |  | <https://pubs.acs.org/doi/pdf/10.1021/ac001246p> |
| 5 | Watson method for getting Hvap at the temperature desired from the BP estimation |  |