

138i Cosmo, Cosmo-Rs, Cosmospace, Cosmotherm, Cosmo-Sac, Cosmo-Rs(OI), Etc.: Definitions, Differences and Comparisons

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By successful academic and industrial applications and by winning the VLE part of the First Industrial Fluid Property Simulation Challenge the quantum chemically based dielectric continuum solvation model COSMO and especially its statistical thermodynamics extension “COSMO for Realistic Solvation” (COSMO-RS) have achieved a considerable degree of interest and recognition. Many researchers in this area consider it as the a breakthrough toward a higher theoretical level for fluid phase thermodynamics, which provides more physical insight and has higher predictive power for demanding chemical compounds than the classical simulation methods, i.e. than the force-field based molecular simulation methods MD and MC and the group contribution methods as UNIFAC.

Since several variants of COSMO-RS have come up during the past years, and since some confusion exists in the literature about the different COSMO related expressions, I will try to give a few important definitions, explain the common features of the different COSMO-RS implementations, and their differences. As far as possible a few quantitative comparisons shall be given as well.