AntÃ³nio J Queimada

List of Publications by Year
in descending order

49 papers	2,874 citations	159358 30 h-index	189595 50 g-index
50 all docs	50 docs citations	50 times ranked	2767 citing authors

#	Article	IF	Citations
1	Modeling of Hydrate Dissociation Curves with a Modified Cubic-Plus-Association Equation of State. Industrial & Engineering Chemistry Research, 2019, 58, 14476-14487.	1.8	4
2	Modeling Hydrate Dissociation Curves in the Presence of Hydrate Inhibitors with a Modified CPA EoS. Industrial & Engineering Chemistry Research, 2019, 58, 19239-19250.	1.8	6
3	Using Volume Shifts To Improve the Description of Speed of Sound and Other Derivative Properties with Cubic Equations of State. Industrial & Engineering Chemistry Research, 2019, 58, 8856-8870.	1.8	2
4	Modeling of the Mixture Critical Locus with a Modified Cubic Plus Association (CPA) EoS: Aromatics, Ketones, Ethers, Diethyl Carbonate, and THF. Industrial & Engineering Chemistry Research, 2018, 57, 15857-15868.	1.8	5
5	Modeling of the Mixture Critical Locus with a Modified Cubic Plus Association Equation of State: Water, Alkanols, Amines, and Alkanes. Industrial & Engineering Chemistry Research, 2018, 57, 10649-10662.	1.8	8
6	Using a Volume Shift in Perturbed-Chain Statistical Associating Fluid Theory To Improve the Description of Speed of Sound and Other Derivative Properties. Industrial & Engineering Chemistry Research, 2018, 57, 11804-11814.	1.8	11
7	Re-evaluating the CPA EoS for improving critical points and derivative properties description. Fluid Phase Equilibria, 2017, 436, 85-97.	1.4	24
8	Evaluating Cubic Plus Association Equation of State Predictive Capacities: A Study on the Transferability of the Hydroxyl Group Associative Parameters. Industrial & Engineering Chemistry Research, 2017, 56, 7086-7099.	1.8	15
9	Improved Prediction of Water Properties and Phase Equilibria with a Modified Cubic Plus Association Equation of State. Industrial & Engineering Chemistry Research, 2017, 56, 15163-15176.	1.8	21
10	Carbon dioxide solubility in aqueous solutions of NaCl: Measurements and modeling with electrolyte equations of state. Fluid Phase Equilibria, 2015, 388, 100-106.	1.4	52
11	Solubilities of hydrofluorocarbons in ionic liquids: Experimental and modelling study. Journal of Chemical Thermodynamics, 2014, 73, 36-43.	1.0	31
12	Solubility of hydrofluorocarbons in phosphonium-based ionic liquids: Experimental and modelling study. Journal of Chemical Thermodynamics, 2014, 79, 184-191.	1.0	24
13	Prediction of the nâ€hexane/water and 1â€octanol/water partition coefficients for environmentally relevant compounds using molecular simulation. AICHE Journal, 2012, 58, 1929-1938.	1.8	44
14	Calculation of drug-like molecules solubility using predictive activity coefficient models. Fluid Phase Equilibria, 2012, 322-323, 48-55.	1.4	17
15	High-pressure solubilities of carbon dioxide in ionic liquids based on bis(trifluoromethylsulfonyl)imide and chloride. Journal of Supercritical Fluids, 2012, 65, 1-10.	1.6	55
16	Solubility of high-value compounds in ethyl lactate: Measurements and modeling. Journal of Chemical Thermodynamics, 2012, 48, 93-100.	1.0	51
17	Predicting hydration Gibbs energies of alkyl-aromatics using molecular simulation: a comparison of current force fields and the development of a new parameter set for accurate solvation data. Physical Chemistry Chemical Physics, 2011, 13, 17384.	1.3	22
18	Modeling Phase Equilibria Relevant to Biodiesel Production: A Comparison of g^E Models, Cubic EoS, EoSâ€“g^E and Association EoS. Industrial & Engineering Chemistry Research, 2011, 50, 2348-2358.	1.8	35

#	Article	IF	Citations
19	Measurement and Prediction of Biodiesel Surface Tensions. Energy & Fuels, 2011, 25, 4811-4817.	2.5	45
20	High-Pressure Biodiesel Density: Experimental Measurements, Correlation, and Cubic-Plus-Association Equation of State (CPA EoS) Modeling. Energy & Fuels, 2011, 25, 3806-3814.	2.5	75
21	Using molecular simulation to predict solute solvation and partition coefficients in solvents of different polarity. Physical Chemistry Chemical Physics, 2011, 13, 9155.	1.3	30
22	Solubility of drug-like molecules in pure organic solvents with the CPA EoS. Fluid Phase Equilibria, 2011, 303, 62-70.	1.4	17
23	Liquidâ€“liquid equilibria for the canola oil biodiesel + ethanol + glycerol system. Fuel, 2011, 90, 2738-2745.	3.4	57
24	Evaluation of the CO2 behavior in binary mixtures with alkanes, alcohols, acids and esters using the Cubic-Plus-Association Equation of State. Journal of Supercritical Fluids, 2011, 55, 876-892.	1.6	71
25	Effect of the Integration Method on the Accuracy and Computational Efficiency of Free Energy Calculations Using Thermodynamic Integration. Journal of Chemical Theory and Computation, 2010, 6, 1018-1027.	2.3	83
26	Molecular simulation of the hydration Gibbs energy of barbiturates. Fluid Phase Equilibria, 2010, 289, 148-155.	1.4	17
27	Water solubility of drug-like molecules with the cubic-plus-association equation of state. Fluid Phase Equilibria, 2010, 298, 75-82.	1.4	18
28	Phase Equilibria of Ester + Alcohol Systems and Their Description with the Cubic-Plus-Association Equation of State. Industrial & Engineering Chemistry Research, 2010, 49, 3452-3458.	1.8	44
29	Temperature and solvent effects in the solubility of some pharmaceutical compounds: Measurements and modeling. European Journal of Pharmaceutical Sciences, 2009, 37, 499-507.	1.9	117
30	Description of the mutual solubilities of fatty acids and water with the CPA EoS. AICHE Journal, 2009, 55, 1604-1613.	1.8	46
31	Phase equilibria of glycerol containing systems and their description with the Cubic-Plus-Association (CPA) Equation of State. Fluid Phase Equilibria, 2009, 280, 22-29.	1.4	85
32	Thermodynamic Modeling of the Aqueous Solubility of PAHs. Industrial & Engineering Chemistry Research, 2009, 48, 5530-5536.	1.8	21
33	Solubilities of Biologically Active Phenolic Compounds: Measurements and Modeling. Journal of Physical Chemistry B, 2009, 113, 3469-3476.	1.2	89
34	1-Octanol/Water Partition Coefficients of n-Alkanes from Molecular Simulations of Absolute Solvation Free Energies. Journal of Chemical Theory and Computation, 2009, 5, 2436-2446.	2.3	115
35	Surface tension of chain molecules through a combination of the gradient theory with the CPA EoS. Fluid Phase Equilibria, 2008, 267, 83-91.	1.4	84
36	Prediction of Water Solubility in Biodiesel with the CPA Equation of State. Industrial & Engineering Chemistry Research, 2008, 47, 4278-4285.	1.8	79

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37	Surface Tensions for the 1-Alkyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide Ionic Liquids. Journal of Chemical & Engineering Data, 2008, 53, 1346-1350.	1.0	199
38	Modeling the Liquidâ"Liquid Equilibria of Water + Fluorocarbons with the Cubic-Plus-Association Equation of State. Industrial & Engineering Chemistry Research, 2007, 46, 1415-1420.	1.8	23
39	Mutual solubilities of hydrocarbons and water with the CPA EoS. Fluid Phase Equilibria, 2007, 258, 58-66.	1.4	140
40	Surface tensions of imidazolium based ionic liquids: Anion, cation, temperature and water effect. Journal of Colloid and Interface Science, 2007, 314, 621-630.	5.0	406
41	Surface Tension of Liquid Fluorocompounds. Journal of Chemical & Engineering Data, 2006, 51, 1820-1824.	1.0	61
42	Prediction of viscosities and surface tensions of fuels using a new corresponding states model. Fuel, 2006, 85, 874-877.	3.4	42
43	Modeling vaporâ€"liquid interfaces with the gradient theory in combination with the CPA equation of state. Fluid Phase Equilibria, 2005, 228-229, 479-485.	1.4	59
44	Viscosity and Liquid Density of Asymmetric n-Alkane Mixtures: Measurement and Modeling. International Journal of Thermophysics, 2005, 26, 47-61.	1.0	79
45	Surface Tension of Decane Binary and Ternary Mixtures with Eicosane, Docosane, and Tetracosane. Journal of Chemical & Engineering Data, 2005, 50, 1043-1046.	1.0	41
46	Viscosity and Liquid Density of Asymmetric Hydrocarbon Mixtures. International Journal of Thermophysics, 2003, 24, 1221-1239.	1.0	83
47	A new Corresponding States model for the estimation of thermophysical properties of long chain n-alkanes. Fluid Phase Equilibria, 2003, 212, 303-314.	1.4	29
48	Measurement and modeling of surface tensions of asymmetric systems: heptane, eicosane, docosane, tetracosane and their mixtures. Fluid Phase Equilibria, 2003, 214, 211-221.	1.4	52
49	Surface Tension of Heptane, Decane, Hexadecane, Eicosane, and Some of Their Binary Mixtures. Journal of Chemical & Engineering Data, 2002, 47, 1442-1445.	1.0	137