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890	Perturbed-Chain-SAFT: development of a new equation of state for simple, associating, multipolar and polymeric compounds. 2004 , 295-322		2
889	Application of the perturbed chain SAFT equation of state to complex polymer systems using simplified mixing rules. 2004 , 215, 71-78		46
888	Applying Association Theories to Polar Fluids. <i>Industrial & amp; Engineering Chemistry Research</i> , 2004 , 43, 1803-1806	3.9	48
887	A novel approach to liquid I quid equilibrium in polymer systems with application to simplified PC-SAFT. 2004 , 222-223, 87-93		27
886	Application of the Perturbed-Chain SAFT equation of state to polar systems. 2004 , 217, 233-239		129
885	Reactive Phase Equilibria in Silica Aerogel Synthesis: Experimental Study and Prediction of the Complex Phase Behavior Using the PC-SAFT Equation of State. <i>Industrial & amp; Engineering Chemistry Research</i> , 2004 , 43, 4457-4464	3.9	30
884	Novel Method for Estimating Pure-Component Parameters for Polymers: Application to the PC-SAFT Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 2830-2838	3.9	49
883	Liquid[liquid Equilibria for Binary and Ternary Polymer Solutions with PC-SAFT. <i>Industrial &</i> Engineering Chemistry Research, 2004 , 43, 1125-1132	3.9	31
882	Application of the Simplified PC-SAFT Equation of State to the Vapor Liquid Equilibria of Binary and Ternary Mixtures of Polyamide 6 with Several Solvents. <i>Industrial & Discrete Engineering Chemistry Research</i> , 2004 , 43, 826-834	3.9	33
881	Density measurements under pressure for the binary system (ethanol+methylcyclohexane). 2005 , 37, 1294-1304		22
880	Phase-equilibrium calculations for non-aqueous and aqueous associating systems using continuous thermodynamics. 2005 , 230, 143-152		10
879	Thermodynamic modeling of complex systems using PC-SAFT. 2005 , 228-229, 89-98		99
878	Volumetric properties under pressure for the binary system ethanol+toluene. 2005 , 235, 139-151		56
877	Modeling of Aqueous Electrolyte Solutions with Perturbed-Chain Statistical Associated Fluid Theory. <i>Industrial & Discourse amp; Engineering Chemistry Research</i> , 2005 , 44, 3355-3362	3.9	213

(2006-2005)

876	Extended statistical associating fluid theory (SAFT) equations of state for dipolar fluids. <i>AICHE Journal</i> , 2005 , 51, 2328-2342	3.6	106
875	Compressed liquid densities and excess volumes of CO2 + thiophene binary mixtures from 313 to 363 K and pressures up to 25 MPa. 2005 , 236, 193-204		25
874	Thermodynamics of Phase and Chemical Equilibrium in a Strongly Nonideal Esterification System. Journal of Chemical & Engineering Data, 2005, 50, 92-101	2.8	35
873	Extension of the Cubic-plus-Association (CPA) Equation of State to Amines. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 4406-4413	3.9	38
872	Prediction and Correlation of High-Pressure Gas Solubility in Polymers with Simplified PC-SAFT. <i>Industrial & Discourse Chemistry Research</i> , 2005 , 44, 3330-3335	3.9	34
871	Evaluation of the Truncated Perturbed Chain-Polar Statistical Associating Fluid Theory for Complex Mixture Fluid Phase Equilibria. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 6063-6074	3.9	64
870	Comparison of Two Association Models (ElliottBureshDonohue and Simplified PC-SAFT) for Complex Phase Equilibria of HydrocarbonWater and Amine-Containing Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 8170-8179	3.9	60
869	A structural phase diagram for model aqueous organic nanodroplets. 2006 , 8, 1266-70		18
868	Application of the Cubic-Plus-Association (CPA) Equation of State to Complex Mixtures with Aromatic Hydrocarbons. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 1527-1538	3.9	97
867	A study of Wertheim's thermodynamic perturbation theory (TPT1) for associating fluids with dispersive interactions: the importance of the association range. 2006 , 104, 3551-3560		12
866	Ten Years with the CPA (Cubic-Plus-Association) Equation of State. Part 2. Cross-Associating and Multicomponent Systems. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 4869-4878	3.9	189
865	Reaction Kinetics of the Homogeneously Catalyzed Esterification of 1-Butanol with Acetic Acid in a Wide Range of Initial Compositions. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 1869-187	7 3 .9	23
864	Investigation of Critical Properties and Surface Tensions for n-Alkanes by Perturbed-Chain Statistical Associating Fluid Theory Combined with Density-Gradient Theory and Renormalization-Group Theory. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 8199-8206	3.9	36
863	Investigation of Vaporliquid Equilibria for Supercritical Carbon Dioxide and Hydrocarbon Mixtures by Perturbed-Chain Statistical Associating Fluid Theory. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 4364-4370	3.9	27
862	Efficient Solution of the Association Term Equations in the Statistical Associating Fluid Theory Equation of State. <i>Industrial & Equation Chemistry Research</i> , 2006 , 45, 6056-6062	3.9	16
861	Developing optimal Wertheim-like models of water for use in Statistical Associating Fluid Theory (SAFT) and related approaches. 2006 , 104, 3561-3581		146
860	Solubility of Amino Acids: Influence of the pH value and the Addition of Alcoholic Cosolvents on Aqueous Solubility. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 6578-6584	3.9	160
859	Vapor liquid equilibrium modeling of alkane systems with Equations of State: Bimplicity versus complexity [2006, 240, 127-139]		45

858	Modeling the thermodynamic behavior of poly(lactide-co-glycolide) + supercritical fluid mixtures with equations of state. 2006 , 244, 16-25		16
857	Volumetric and derivative properties under pressure for the system 1-propanol+toluene: A discussion of PC-SAFT and SAFT-VR. 2006 , 247, 121-134		63
856	Ten Years with the CPA (Cubic-Plus-Association) Equation of State. Part 1. Pure Compounds and Self-Associating Systems. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 4855-4868	3.9	301
855	Phase equilibria in polydisperse and associating copolymer solutions: Poly(ethene-co-(meth)acrylic acid) thonomer mixtures. 2006 , 241, 113-123		48
854	Capabilities, limitations and challenges of a simplified PC-SAFT equation of state. 2006 , 241, 344-353		41
853	Comparative experimental and modeling studies of the viscosity behavior of ethanol + C7 hydrocarbon mixtures versus pressure and temperature. 2006 , 245, 6-19		38
852	An equation of state contribution for polar components: Polarizable dipoles. <i>AICHE Journal</i> , 2006 , 52, 1951-1961	3.6	96
851	Theoretical Prediction of Thermal Diffusion in WaterMethanol, WaterEthanol, and WaterEsopropanol Mixtures using the PC-SAFT Equation of State. 2006 , 31,		14
850	On the estimation of water pure compound parameters in association theories. 2007 , 105, 1797-1801		18
849	Phase equilibrium of liquid mixtures: experimental and modeled data using statistical associating fluid theory for potential of variable range approach. 2007 , 127, 144513		9
848	Theoretical approach to evaluate thermodiffusion in aqueous alkanol solutions. 2007 , 126, 014502		27
847	PC-SAFT Equation of State Applied to Petroleum Reservoir Fluids. 2007,		17
846	A comprehensive description of chemical association effects on second derivative properties of alcohols through a SAFT-VR approach. 2007 , 111, 3447-61		76
845	Thermodynamic Modeling of the Water + Acetic Acid + CO2System: ☐The Importance of the Number of Association Sites of Water and of the Nonassociation Contribution for the CPA and SAFT-Type Models. <i>Industrial & Description of the Models and Saft-Type Models. Industrial & Description of the Models and Saft-Type Models. Industrial & Description of the Material & Des</i>	3.9	38
844	ThermoData Engine (TDE): software implementation of the dynamic data evaluation concept. 2. Equations of state on demand and dynamic updates over the web. 2007 , 47, 1713-25		54
843	Homogeneous Binary Nucleation Theory and the Structure of Binary Nanodroplets. 2007 , 267-277		2
842	Use of PC-SAFT for Global Phase Diagrams in Binary Mixtures Relevant to Natural Gases. 3. Alkane + Non-Hydrocarbons. <i>Industrial & Engineering Chemistry Research</i> , 2007 , 46, 291-296	3.9	12
841	Phase equilibrium of binary mixtures of cyclic ethers + chlorobutane isomers: experimental measurements and SAFT-VR modeling. 2007 , 111, 9588-97		16

(2008-2007)

840	Associating Fluid Theory Combined with Density-Gradient Theory. <i>Industrial & amp; Engineering</i> 3.9 Chemistry Research, 2007 , 46, 7378-7383	28
839	tPC-PSAFT Modeling of Gas Solubility in Imidazolium-Based Ionic Liquids 2007, 111, 15487-15492	88
838	Modeling of Polar Systems Using PCP-SAFT: An Approach to Account for Induced-Association Interactions 2007, 111, 15544-15553	121
837	Genetic algorithm for the determination of binodal curves in ternary systems polymer-liquid(1)-liquid(2) and polymer(1)-polymer(2)-solvent. 2007 , 28, 2203-15	9
836	Modeling vaporliquid equilibria of ethanol+1,1,1,2,3,3,3-heptafluoropropane binary mixtures using PC-SAFT. 2007 , 260, 190-194	15
835	Modeling of solid[Iquid equilibria for systems with solid-complex phase formation. 2007 , 260, 98-104	38
834	Continuous thermodynamics of binary associating systems. 2007 , 254, 174-187	5
833	Measurement and modelling of hydrogen bonding in 1-alkanol+n-alkane binary mixtures. 2007 , 261, 272-280	28
832	Modelling of associating mixtures for applications in the oil & gas and chemical industries. 2007 , 261, 205-211	34
831	A semi-empirical hard-sphere chain equation of state: Pure and mixture. 2007 , 261, 258-264	4
830	An evaluation of the performance of the Cubic-Plus-Association equation of state in mixtures of non-polar, polar and associating compounds: Towards a single model for non-polymeric systems. 2007 , 261, 343-350	36
829	Application of the PC-SAFT equation of state to modeling of solid-liquid equilibria in systems with organic components forming chemical compounds. 2007 , 80, 542-548	17
828	Phase equilibria in water containing binary systems from molecular based equations of state. 2007 , 254, 112-125	49
827	Modeling phase equilibria of alkanols with the simplified PC-SAFT equation of state and generalized pure compound parameters. 2007 , 258, 83-94	65
826	Experimental investigation and prediction of oiling out during crystallization process. 2008, 310, 4163-4168	57
825	Isothermal (vapour + liquid) equilibrium of (cyclic ethers + chlorohexane) mixtures: Experimental results and SAFT modelling. 2008 , 40, 1253-1260	6
824	Calculation of critical points for multicomponent mixtures containing hydrocarbon and nonhydrocarbon components with the PC-SAFT equation of state. 2008 , 265, 192-204	22
823	Modeling of aqueous amino acid and polypeptide solutions with PC-SAFT. 2008 , 47, 1018-1025	91

822	A Predictive Group-Contribution Simplified PC-SAFT Equation of State: Application to Polymer Systems. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 5092-5101	3.9	134
821	Supercritical Fluids. 2008,		
820	Investigation of Vaporlliquid Surface Tension for Carbon Dioxide and Hydrocarbon Mixtures by Perturbed-Chain Statistical Associating Fluid Theory Combined with Density-Gradient Theory. <i>Industrial & Density Engineering Chemistry Research</i> , 2008 , 47, 4490-4495	3.9	49
819	Measurements and predictive models for the N-methyl-2-pyrrolidone/water/methanol system. 2008 , 112, 11361-73		38
818	Phase Equilibrium Modelling for Mixtures with Acetic Acid Using an Association Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 5660-5668	3.9	28
817	Calculation of Solubility Parameter Using Perturbed-Chain SAFT and Cubic-Plus-Association Equations of State. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 9663-9669	3.9	18
816	Setup and Validation of a PII Measuring Device. Volumetric Behavior of the Mixture 1,8-Cineole + Ethanol. <i>Journal of Chemical & Description (Chemical & Data)</i> 1393-1400	2.8	23
815	JouleThomson Inversion Curves and Third Virial Coefficients for Pure Fluids from Molecular-Based Models. <i>Industrial & Discourt Amp; Engineering Chemistry Research</i> , 2008 , 47, 8894-8905	3.9	26
814	Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-ChainBtatistical Associating Fluid Theory (sPC-SAFT). 1. Vaporliquid Equilibria. <i>Industrial & Digineering Chemistry Research</i> , 2008 , 47, 5636-5650	3.9	59
813	Renormalization-Group Corrections to a Perturbed-Chain Statistical Associating Fluid Theory for Pure Fluids Near to and Far from the Critical Region. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 6264-6274	3.9	32
812	Evaluation of the Nonrandom Hydrogen Bonding (NRHB) Theory and the Simplified Perturbed-Chain@tatistical Associating Fluid Theory (sPC-SAFT). 2. Liquid@iquid Equilibria and Prediction of Monomer Fraction in Hydrogen Bonding Systems. Industrial & Company &	3.9	57
811	Investigation of Interfacial Tensions for Carbon Dioxide Aqueous Solutions by Perturbed-Chain Statistical Associating Fluid Theory Combined with Density-Gradient Theory. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 8911-8917	3.9	49
810	Thermodynamics of Polymer Solutions. 2008 , 499-537		
809	Solvation Phenomena in Association Theories with Applications to Oil & Gas and Chemical Industries. 2008 , 63, 305-319		39
808	A new approach to evaluate the thermodiffusion factor for associating mixtures. 2009 , 130, 064506		11
807	Vaporliquid equilibrium in the n-butane+methanol system, measurement and modeling from 323.2 to 443.2K. 2009 , 277, 152-161		24
806	Investigation of the surface tension of methane and n-alkane mixtures by perturbed-chain statistical associating fluid theory combined with density-gradient theory. 2009 , 279, 136-140		33
805	Vapor I lquid equilibrium measurements and modeling of the n-butane + ethanol system from 323 to 423 K. 2009 , 286, 79-87		15

(2010-2009)

804	Phase equilibria of carbon dioxide + poly ethylene glycol + water mixtures at high pressure: Measurements and modelling. 2009 , 286, 162-169	20
803	Application of sPC-SAFT and group contribution sPC-SAFT to polymer systems@apabilities and limitations. 2009 , 281, 70-77	20
802	Thermodynamic Modeling of Several Aqueous Alkanol Solutions Containing Amino Acids with the Perturbed-Chain Statistical Associated Fluid Theory Equation of State. <i>Industrial & amp; Engineering Ghemistry Research</i> , 2009 , 48, 5498-5505	13
801	Investigation of Bulk and Interfacial Properties for Nitrogen and Light Hydrocarbon Binary Mixtures by Perturbed-Chain Statistical Associating Fluid Theory Combined with Density-Gradient Theory. 3.9 Industrial & Samp; Engineering Chemistry Research, 2009, 48, 10734-10739	27
800	Phase Behavior Modeling of Alkyl Amine + Hydrocarbon and Alkyl Amine + Alcohol Systems Using a Group Contribution Associating Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 3.9 2009 , 48, 7705-7712	14
799	Effect of Gas Impurities on the Throttling Process of Fluorocarbon Refrigerants: Estimation of the Henry Law Constant. <i>Journal of Chemical & Engineering Data</i> , 2009 , 54, 2395-2403	14
798	Modeling the phase equilibria of hydrogen sulfide and carbon dioxide in mixture with hydrocarbons and water using the PCP-SAFT equation of state. 2010 , 293, 11-21	59
797	Are safe results obtained when the PC-SAFT equation of state is applied to ordinary pure chemicals?. 2010 , 295, 76-92	109
796	Equation of state for aqueous electrolyte systems based on the semirestricted non-primitive mean spherical approximation. 2010 , 297, 23-33	28
795	Thermophysical properties of the binary mixtures (1,8-cineole + 1-alkanol) at $T = (298.15 \text{ and } 313.15)$ K and at atmospheric pressure. 2010 , 42, 291-303	36
794	Bulk and Interfacial Properties for CO2-SO2 Binary Mixtures. 2010 , 28, 1885-1889	4
793	Transferable intermolecular potentials for carboxylic acids and their phase behavior. <i>AICHE Journal</i> , 2010 , 56, NA-NA	5
792	Selbst- und Kreuzassoziation in Mischungen. 2010 , 82, 1376-1377	
791	Phase equilibria modeling of methanol-containing systems with the CPA and sPC-SAFT equations of state. 2010 , 288, 128-138	27
790	Use of monomer fraction data in the parametrization of association theories. 2010 , 296, 219-229	49
789	☑aporŪquidଢquilibrium measurements and modeling for the cyclohexane + cyclohexanol binary system. 2010 , 298, 33-37	5
788	pePC-SAFT: Modeling of polyelectrolyte systems. 2010 , 299, 84-93	12
787	Thermodynamic modeling of CO2 solubility in aqueous solutions of NaCl and Na2SO4. 2010 , 55, 623-634	47

786	Interfacial properties of mixtures containing supercritical gases. 2010 , 55, 724-734	72
785	Density functional theory for calculating surface tensions with a simple renormalization formalism for the critical point. 2010 , 55, 735-742	23
7 ⁸ 4	Equation of state modeling of high-pressure, high-temperature hydrocarbon density data. 2010 , 55, 701-71	1 71
7 ⁸ 3	Compatible solutes: Thermodynamic properties and biological impact of ectoines and prolines. 2010 , 152, 28-39	73
782	Modelling LLE and VLE of methanol+n-alkane series using GC-PC-SAFT with a group contribution kij. 2010 , 298, 154-168	53
781	Solubility calculation of pharmaceutical compounds (A) priori parameter estimation using quantum-chemistry. 2010 , 299, 161-170	23
780	Phase behavior of the system hyperbranched polyglycerol+methanol+carbon dioxide. 2010 , 299, 252-258	15
779	Vaporliquid Equilibria of Acid GasAqueous Ethanolamine Solutions Using the PC-SAFT Equation of State. <i>Industrial & Damp; Engineering Chemistry Research</i> , 2010 , 49, 7620-7630	57
778	BACK MATTER. 2010 , 207-260	
777	Modeling of Vaporliquid Equilibria for CO2 + 1-Alkanol Binary Systems with the PC-SAFT Equation of State Using Polar Contributions Industrial & Engineering Chemistry Research, 2010, 49, 12276-12283	14
776	P, []T Measurements and Isobaric Vapor [liquid Equilibria of the 1,3,3-Trimethyl-2-oxabicycle [2,2,2] octane + Propan-1-ol Mixture: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analysis. <i>Journal of Chemical & Data</i> , 2010,	10
775	PI Measurements of the (Ethanol + Linalool), (Propan-1-ol + Linalool), and (Propan-2-ol + Linalool) Mixtures: Cubic and Statistical Associating Fluid Theory-Based Equation of State Analyses. <i>Journal</i> 2.8 of Chemical & Camp; Engineering Data, 2010 , 55, 5332-5339	11
774	Application of Infinite Dilution Activity Coefficients for Determining Binary Equation of State Parameters. <i>Industrial & Determining Chemistry Research</i> , 2010 , 49, 7646-7653	15
773	Calculation of Pressure II emperature Diagrams and Distance for Phase Transition in Polyethylene Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 12242-12253	7
772	A simplified Van der Waals-Platteeuw model of clathrate hydrates with multiple occupancy of cavities. 2010 , 114, 9602-7	26
771	An Object-Oriented Approach for Structure Design of Property Calculation Programs Using Equations of State. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 6404-6412	O
770	P, □and T Measurements of the Limonene + ⊞-Pinene Mixtures. <i>Journal of Chemical & Data & 2011</i> , 56, 1709-1713	4
769	Isothermal Vaporliquid Equilibrium of (1-Butanol + 1,8-Cineole) at 10 Temperatures between (278.15 and 323.15) K. <i>Journal of Chemical & Data</i> , 2011, 56, 2443-2448	7

(2011-2011)

768	Vaporlliquid Equilibrium Calculations of Aqueous and Nonaqueous Binary Systems Using the Mattedillavares astier Equation of State. <i>Industrial & Discourse Engineering Chemistry Research</i> , 2011 , 50, 102-110	3.9	2
767	Transferable SAFT-VR models for the calculation of the fluid phase equilibria in reactive mixtures of carbon dioxide, water, and n-alkylamines in the context of carbon capture. 2011 , 115, 8155-68		69
766	Measurement and modeling of CO2 solubility in NaCl brine and CO2Baturated NaCl brine density. 2011 , 5, 1460-1477		116
765	Solubility of Ethene in Water and in a Medium for the Cultivation of a Bacterial Strain. <i>Journal of Chemical & Engineering Data</i> , 2011 , 56, 1596-1601	2.8	4
764	Measuring and Modeling Activity Coefficients in Aqueous Amino-Acid Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 131-141	3.9	109
763	Modeling Gas Solubilities in the Aqueous Solution of Methyldiethanolamine. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 6436-6446	3.9	19
762	Thermodynamic Modeling for CO2 Absorption in Aqueous MDEA Solution with Electrolyte NRTL Model. <i>Industrial & Discourse Engineering Chemistry Research</i> , 2011 , 50, 163-175	3.9	125
761	Solubility of aliphatic hydrocarbons in piperidinium ionic liquids: measurements and modeling in terms of perturbed-chain statistical associating fluid theory and nonrandom hydrogen-bonding theory. 2011 , 115, 12537-48		47
760	Modeling pH and Solubilities in Aqueous Multisolute Amino Acid Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 3503-3509	3.9	41
759	Modeling Liquid l iquid and Liquid l 'apor Equilibria of Binary Systems Containing Water with an Alkane, an Aromatic Hydrocarbon, an Alcohol or a Gas (Methane, Ethane, CO2or H2S), Using Group Contribution Polar Perturbed-Chain Statistical Associating Fluid Theory. <i>Industrial & Description</i> 100 March 100	3.9	73
75 ⁸	Behavior of the Environmentally Compatible Absorbent 1-Butyl-3-methylimidazolium Tetrafluoroborate with 2,2,2-Trifluoroethanol: Experimental Densities at High Pressures and Modeling of PVT and Phase Equilibria Behavior with PC-SAFT EoS. <i>Industrial & Engineering</i>	3.9	19
757	Chemistry Research, 2011 , 50, 4065-4076 THERMOPHYSICAL PROPERTIES OF ASSOCIATING FLUIDS IN NATURAL GAS INDUSTRY USING PC-SAFT EQUATION OF STATE. 2011 , 198, 1244-1262		6
756	Cross-Association Model for the Phase Equilibria and Surface Tensions of CO2Methanol and CO2Ethanol Mixtures. 2011 , 115, 3340-3345		4
755	Minimal Experimental Data Set Required for Estimating PCP-SAFT Parameters. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 11746-11754	3.9	14
754	New Association Scheme for 1-Alcohols in Alcohol/Water Mixtures with sPC-SAFT: The 2C Association Scheme. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 8711-8725	3.9	23
753	Thermodynamic Modeling of the NH3©O2H2O System with Electrolyte NRTL Model. <i>Industrial</i> & Samp; Engineering Chemistry Research, 2011 , 50, 11406-11421	3.9	64
752	Modeling of the Thermodynamics of the Acetic Acid Water Mixture Using the Cubic-Plus-Association Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 57	793-380)5 ²⁰
751	Determining force field parameters using a physically based equation of state. 2011 , 115, 7872-80		31

75°	Solubility of nitrogen in one-component refrigerants: Prediction by PC-SAFT EoS and a correlation of Henry law constants. 2011 , 34, 2109-2117		19
749	Thermophysical behaviour of the mixture (⊞)-3,7-dimethyl-1,6-octadien-3-ol with ethanol. 2011 , 308, 78-89		13
748	☑aporŪquidଢ️quilibrium measurements and modeling for the cyclohexane+n-hexanoic acid binary system. 2011 , 309, 15-19		1
747	Experimental measurements and equation of state modeling of liquid densities for long-chain n-alkanes at pressures to 265MPa and temperatures to 523K. 2011 , 311, 17-24		45
746	Thermodynamic modeling for CO2 absorption in aqueous MEA solution with electrolyte NRTL model. 2011 , 311, 67-75		115
745	Phase behavior of hyperbranched polymer solutions in mixed solvents. <i>Chemical Engineering Science</i> , 2011 , 66, 5244-5252	4.4	35
744	Using an Analytic Equation of State to Obtain Quantitative Solubilities of CO2 by Molecular Simulation. 2011 , 2, 393-396		6
743	Phase- and interfacial behavior of hyperbranched polymer solutions. 2011 , 302, 321-330		46
742	Thermodynamic modeling of CO2 and H2S solubilities in aqueous DIPA solution, aqueous sulfolane DIPA solution, and aqueous sulfolane DIPA solution with electrolyte NRTL model. 2011 , 306, 190-203		56
741	20 Years of the SAFT equation of state R ecent advances and challenges: Symposium held in Bellaterra, Barcelona, 19 1 1 September 2010. 2011 , 306, 1-3		20
740	Modeling of solid[Iquid equilibria for polyethylene and polypropylene solutions with equations of state. 2011 , 121, 1832-1849		9
739	Thermodynamische Berechnungsmethoden f Lalichkeiten. 2011 , 83, 496-502		6
738	Thermodynamics of pharmaceuticals: Prediction of solubility in pure and mixed solvents with PC-SAFT. 2011 , 302, 331-337		42
737	Equation of state for square-well chain molecules with variable range, extension to associating fluids. 2011 , 302, 139-152		5
736	Calculation of surface tension of metals using density gradient theory and PC-SAFT equation of state. 2011 , 301, 13-17		9
735	Integration of process and solvent design towards a novel generation of CO2 absorption capture systems. 2011 , 4, 282-290		17
734	Prediction of multiphase equilibrium using the PC-SAFT equation of state and simultaneous testing of phase stability. 2011 , 302, 169-178		22
733	An equation of state for acetic acid including the association term of SAFT. 2011 , 303, 134-149		7

732	SolidIlquid equilibrium using the SAFT-VR equation of state: Solubility of naphthalene and acetic acid in binary mixtures and calculation of phase diagrams. 2011 , 306, 137-147		8
731	pePC-SAFT: Modeling of polyelectrolyte systems 2. Aqueous two-phase systems. 2011 , 306, 67-75		10
730	Liquid II quid phase equilibrium of (piperidinium-based ionic liquid+an alcohol) binary systems and modelling with NRHB and PCP-SAFT. 2011 , 305, 43-52		64
729	Thermophysical properties of {(日)-linalool+propan-1-ol}: A first stage towards the development of a green process. 2011 , 43, 527-536		17
728	Experimental study and PC-SAFT simulations of sorption equilibria in polystyrene. 2011 , 52, 3082-3091		12
727	Density-functional theory for polymer-carbon dioxide mixtures: a perturbed-chain SAFT approach. 2012 , 137, 054902		37
726	Cross-association of multi-component systems. 2012 , 110, 1249-1260		12
725	GEM-SELEKTOR GEOCHEMICAL MODELING PACKAGE: TSolMod LIBRARY AND DATA INTERFACE FOR MULTICOMPONENT PHASE MODELS. 2012 , 50, 1173-1195		268
724	Modeling imidazolium-based ionic liquids with ePC-SAFT. 2012 , 335, 64-73		104
723	Vapourliquid equilibrium of binary systems containing pentafluorochemicals from 363 to 413 K: Measurement and modelling with PengRobinson and three SAFT-like equations of states. 2012 , 35, 2297-2310		13
722	Hydroformylation of 1-Dodecene in the Thermomorphic Solvent System Dimethylformamide/Decane. Phase BehaviorReaction PerformanceLatalyst Recycling. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 10296-10306	3.9	102
721	Approach to Improve Speed of Sound Calculation within PC-SAFT Framework. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 14903-14914	3.9	55
720	Modeling Liquid Liquid Equilibria of Polyimide Solutions. <i>Industrial & Discourse Industrial & Discourse Industrial & Discours Industrial & Discourse Industrial</i>	3.9	24
719	Influence of cyclic dimer formation on the phase behavior of carboxylic acids. 2012 , 116, 7874-82		18
718	Heterosegmented Perturbed-Chain Statistical Associating Fluid Theory as a Robust and Accurate Tool for Modeling of Various Alkanes. 1. Pure Fluids. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 12967-12983	3.9	28
717	Liquid Liquid Equilibria of Systems with Linear Aldehydes. Experimental Data and Modeling with PCP-SAFT. <i>Industrial & amp; Engineering Chemistry Research</i> , 2012 , 51, 14525-14534	3.9	18
716	Modeling Poly(N-isopropylacrylamide) Hydrogels in Water/Alcohol Mixtures with PC-SAFT. 2012 , 45, 6686-6696		49
715	VOC sorption in glassy polyimides™easurements and modeling. 2012 , 415-416, 596-607		12

714	Reducing the amount of PCP-SAFT fitting parameters. 1. Non-polar and dipolar components. 2012 , 326, 21-30		12
713	Reducing the amount of PCPBAFT fitting parameters. 2. Associating components. 2012 , 326, 31-44		18
712	Testing the ability of various equations of state to reproduce high-pressure isotherm crossings in the (\mathbb{H} , P) plane. 2012 , 327, 45-57		7
711	Thermodynamic properties and vaporliquid equilibria of associating fluids, Peng R obinson equation of state coupled with shield-sticky model. 2012 , 330, 1-11		2
710	Phase equilibrium and interfacial properties of water + CO2 mixtures. 2012 , 332, 40-47		45
709	Development of an EOS based on lattice cluster theory for pure components. 2012 , 331, 58-79		18
708	Experimental determination of the critical loci for {n-C6H14 or CO2+alkan-1-ol} mixtures. Evaluation of their critical and subcritical behavior using PC-SAFT EoS. 2012 , 71, 26-44		39
707	Environmental Resistance of High Performance Polymeric Matrices and Composites. 2012 , 1		4
706	Modeling the phase equilibria of a H2OLO2 mixture with PC-SAFT and tPC-PSAFT equations of state. 2012 , 110, 1205-1212		36
705	Vaporliquid Equilibrium at p/kPa = 101.3 of the Binary Mixtures of Ethenyl Acetate with Methanol and Butan-1-ol. <i>Journal of Chemical & Engineering Data</i> , 2012 , 57, 3198-3202	2.8	3
704	Perturbed-chain SAFT as a versatile tool for thermodynamic modeling of binary mixtures containing isoquinolinium ionic liquids. 2012 , 116, 8191-200		31
703	A Survey of Equations of State for Polymers. 2012 ,		6
702	Osmotic coefficients of aqueous weak electrolyte solutions: influence of dissociation on data reduction and modeling. 2012 , 116, 7479-91		19
701	Thermodynamic modeling of ionic liquid systems: development and detailed overview of novel methodology based on the PC-SAFT. 2012 , 116, 5002-18		88
700	Correlation of solubility of single gases/hydrocarbons in polyethylene using PC-SAFT. 2012 , 7, 406-417		9
699	Measuring and modeling alcohol/salt systems. <i>Chemical Engineering Science</i> , 2012 , 68, 328-339	4.4	58
698	Thermodynamics of water sorption in poly(e-caprolactone): A comparative analysis of lattice fluid models including hydrogen bond contributions. 2012 , 313, 127-139		16
697	Prediction of hydrocarbon densities at extreme conditions using volume-translated SRK and PR equations of state fit to high temperature, high pressure PVT data. 2012 , 317, 65-76		65

696	Are safe results obtained when SAFT equations are applied to ordinary chemicals? Part 2: Study of solid[]quid equilibria in binary systems. 2012 , 318, 61-76	35
695	High temperature-high pressure density prediction of hydrocarbon systems using an extended LJ potential-based equation of state. 2012 , 68, 71-80	5
694	P, [land T measurements of the (limonene + 即inene) mixtures. 2012 , 48, 175-180	1
693	Impact of density gradients on the fluid flow inside a vibrating cavity subjected to soret effect. 2013 , 91, 550-559	10
692	Phase behavior of reservoir fluids: Comparisons of PC-SAFT and cubic EOS simulations. 2013 , 359, 17-23	32
691	Phase behavior of sour natural gas systems using classical and statistical thermodynamic equations of states. 2013 , 356, 136-145	12
690	Association theories for complex thermodynamics. 2013 , 91, 1840-1858	29
689	Calculations of Complex Phase Equilibrium by Semigrand Canonical Ensemble. <i>Industrial & amp;</i> Engineering Chemistry Research, 2013 , 52, 9690-9697 3-9	
688	Liquid Liquid Equilibria of 1-Butanol/Water/IL Systems. <i>Industrial & Description of Systems of Sys</i>	77
687	Integrierte chemische Prozesse in fl\u00dfsigen Mehrphasensystemen. 2013, 85, n/a-n/a	
686	Modeling induced nucleation processes during batch cooling crystallization: A sequential parameter determination procedure. 2013 , 52, 216-229	41
685	Modelling of organic-solvent flux through a polyimide membrane. 2013 , 428, 554-561	27
684	Influence of methane and carbon monoxide in the volumetric behaviour of the anthropogenic CO2: Experimental data and modelling in the critical region. 2013 , 18, 264-276	9
683	Prediction of the vaporliquid equilibria and speed of sound in binary systems of 1-alkanols and n-alkanes with the simplified PC-SAFT equation of state. 2013 , 360, 222-232	36
682	Effect of isomeric structures of branched cyclic hydrocarbons on densities and equation of state predictions at elevated temperatures and pressures. 2013 , 117, 8821-30	5
681	Intelligent Hydrogels. 2013,	9
<i>6</i> 80	Classical density functional theory for associating fluids in orienting external fields. 2013, 88, 060301	7
679	Equations of State and Formulations for Mixtures. 2013 , 333-480	2

678	Simulation on thermodynamic state of ammonia carbonation at low temperature and low pressure. 2013 , 7, 447-455		3
677	A novel continuous flow apparatus with a video camera system for high pressure phase equilibrium measurements. 2013 , 356, 291-300		6
676	Extension of the PC-SAFT based group contribution method for polymers to aromatic, oxygen- and silicon-based polymers. 2013 , 339, 89-104		16
675	Boyle temperature from SAFT, PC-SAFT and SAFT-VR equations of state. <i>Journal of Molecular Liquids</i> , 2013 , 187, 114-128	6	14
674	Measurements of H2S solubility in aqueous diisopropanolamine solutions and vapour pressure of diisopropanolamine. 2013 , 338, 164-171		17
673	Experimental determination and theoretical modeling of the vapor I quid equilibrium and densities of the binary system butan-2-ol+tetrahydro-2H-pyran. 2013 , 342, 52-59		1
672	Evaluation of the PC-SAFT, SAFT and CPA equations of state in predicting derivative properties of selected non-polar and hydrogen-bonding compounds. 2013 , 338, 1-15		69
671	Modeling CO2 solubility in Aqueous Methyldiethanolamine Solutions by Perturbed Chain-SAFT Equation of State. 2013 , 59, 214-221		24
670	PII measurements and derived properties of liquid 1,2-alkanediols. 2013 , 57, 137-144		25
669	High-pressure gas solubility in multicomponent solvent systems for hydroformylation. Part I: Carbon monoxide solubility. 2013 , 81, 23-32		24
668	Thermodynamic modeling of PVTx properties for several water/hydrocarbon systems in near-critical and supercritical conditions. 2013 , 30, 201-212		3
667	Molecular interactions in 1-butanol + IL solutions by measuring and modeling activity coefficients. 2013 , 117, 3173-85		37
666	Excess enthalpies of mixing of piperidinium ionic liquids with short-chain alcohols: measurements and PC-SAFT modeling. 2013 , 117, 3884-91		38
665	Prediction of hydrocarbon densities using an artificial neural networkgroup contribution method up to high temperatures and pressures. 2013 , 556, 89-96		23
664	Evaluation of Cubic, SAFT, and PC-SAFT Equations of State for the Vaporlliquid Equilibrium Modeling of CO2 Mixtures with Other Gases. <i>Industrial & Engineering Chemistry Research</i> , 2013 , 52, 3933-3942	3.9	78
663	Renewable feedstocks in green solvents: thermodynamic study on phase diagrams of D-sorbitol and xylitol with dicyanamide based ionic liquids. 2013 , 117, 7034-46		27
662	P, ☐T and heat capacity measurements of (⊞-pinene + ∰inene) mixtures over the temperature range 283.15 K to 358.15 K and pressures up to 40 MPa: Experiments and modelling. 2013 , 57, 493-499		6
661	Solubility of Pharmaceuticals and Their Salts As a Function of pH. <i>Industrial & Description of the Managery of the Managery Research</i> , 2013 , 52, 2721-2731	3.9	57

660	Bweet-in-Green Bystems Based on Sugars and Ionic Liquids: New Solubility Data and Thermodynamic Analysis. <i>Industrial & Engineering Chemistry Research</i> , 2013 , 52, 18482-18491	9	20
659	An equation of state for methanol including the association term of SAFT. 2013 , 349, 12-24		6
658	Influence of cyclic dimer formation on the phase behavior of carboxylic acids. II. Cross-associating systems. 2013 , 117, 9430-8		13
657	Phase Equilibria for CO2-Ethanol Mixtures by Perturbed-Chain Statistical Associating Fluid Theory. 2013 , 411-414, 2979-2982		O
656	Interfacial Properties for MEA and MEA-Water Mixtures. 2013, 765-767, 3166-3169		
655	Size distribution of associated clusters in liquid alcohols: interpretation of simulation results in the frame of SAFT approach. 2013 , 139, 174502		8
654	Simultane Modellierung von Phasengleichgewichten und Grenzfl\(\mathbb{D}\)heneigenschaften mithilfe des PCP-SAFT-Modells. 2013 , 85, n/a-n/a		2
653	Phase Equilibria and Surface Tensions for MDEA, DEA and their Aqueous Solutions. 2013 , 781-784, 2554-2	559	
652	Performance of predictive models in phase equilibria of complex associating systems: PC-SAFT and CEOS/GE. 2013 , 30, 75-82		1
651	Cluster perturbation theory for the self-assembly of associating fluids into complex structures. 2014 , 90, 062316		3
650	Simha-Somcynsky Equation of State Modeling of the PVT Behavior of PP/Clay-Nanocomposite/CO2 Mixtures. 2014 , 29, 430-439		
649	PC-SAFT parameters from ab initio calculations. 2014 , 362, 41-50		21
648	Model-based prediction of optimal conditions for 1-octene hydroformylation. <i>Chemical Engineering Science</i> , 2014 , 115, 58-68	4	7
647	The role of monomer fraction data in association theories can we improve the performance for phase equilibrium calculations?. 2014 , 365, 112-122		13
646	Modeling the phase behavior of cyclic compounds in mixtures of water, alcohols and hydrocarbons. 2014 , 361, 143-154		13
645	Calculation of complex phase equilibria of DMF/alkane systems using the PCP-SAFT equation of state. <i>Chemical Engineering Science</i> , 2014 , 115, 49-57	4	21
644	New formulation of the lattice cluster theory equation of state for multi-component systems. 2014 , 362, 196-212		15
643	Modeling aqueous two-phase systems: I. Polyethylene glycol and inorganic salts as ATPS former. 2014 , 368, 91-103		41

642	Modelling polylactide/water/dioxane systems for TIPS scaffold fabrication. 2014, 374, 1-8		9
641	Vapor Diquid Equilibria of Water + Alkylimidazolium-Based Ionic Liquids: Measurements and Perturbed-Chain Statistical Associating Fluid Theory Modeling. <i>Industrial & amp; Engineering Chemistry Research</i> , 2014 , 53, 3737-3748	3.9	69
640	Thermodynamic properties of HFO-1243zf and their application in study on a refrigeration cycle. 2014 , 70, 1-6		39
639	High-pressure gas solubility in multicomponent solvent systems for hydroformylation. Part II: Syngas solubility. 2014 , 88, 74-84		18
638	Predicting the Extraction Behavior of Pharmaceuticals. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 865-870	3.9	3
637	Thermophysical properties of {R-fenchone+ethanol} at several temperatures and pressures. 2014 , 69, 48-55		6
636	Thermodynamic properties of binary mixtures containing N,N-dimethylformamide+2-alkanol: Cubic and statistical associating fluid theory-based equation of state analysis. 2014 , 45, 365-371		4
635	Interfacial tension of binary mixtures exhibiting azeotropic behavior: Measurement and modeling with PCP-SAFT combined with Density Gradient Theory. 2014 , 362, 151-162		38
634	Thermodynamic Properties of Binary Mixtures Containing N,N-Dimethylacetamide + 2-Alkanol: Experimental Data and Modeling. <i>Journal of Chemical & Experimental Data</i> , 2014 , 59, 275-281	2.8	23
633	Densities and viscosities of the mixtures (formamide+2-alkanol): Experimental and theoretical approaches. 2014 , 69, 101-106		18
632	Continuous Molecular TargetingLomputer-Aided Molecular Design (CoMTLAMD) for Simultaneous Process and Solvent Design for CO2 Capture. <i>Industrial & Design For Co2 Capture Industrial & Industrial & Design For Co2 Capture Industrial & Design For Co2 Capture</i>	3.9	60
631	Influence of copolymer composition on the phase behavior of solid dispersions. 2014 , 11, 4189-98		62
630	Cellulose and hemicellulose valorisation: an integrated challenge of catalysis and reaction engineering. 2014 , 7, 2803		219
629	Molecular separation with organic solvent nanofiltration: a critical review. 2014 , 114, 10735-806		935
628	Vaporliquid Phase Equilibria and Excess Thermal Properties of Binary Mixtures of Ethylsulfate-Based Ionic Liquids with Water: New Experimental Data, Correlations, and Predictions. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 18316-18325	3.9	25
627	Discussion of the influence of CO and CH4 in CO2 transport, injection, and storage for CCS technology. 2014 , 48, 10984-92		16
626	Modeling Water Containing Systems with the Simplified PC-SAFT and CPA Equations of State. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 14493-14507	3.9	65
625	In silico design of solvents for carbon capture with simultaneous optimisation of operating conditions. 2014 , 30, 179-187		7

624	Modeling of Liquid Interfacial Properties of Binary and Ternary Mixtures. <i>Journal of Chemical & Data</i> , 2014 , 59, 3003-3016	2.8	24
623	Architectural Effects on the Solution Behavior of Linear and Star Polymers in Propane at High Pressures. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 10133-10143	3.9	8
622	Evaluation of thermodynamic properties of fluid mixtures by PC-SAFT model. 2014 , 591, 75-80		17
621	High-Pressure Densities of 2,2,2-Trifluoroethanol + Ionic Liquid Mixtures Useful for Possible Applications in Absorption Cycles. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 10791-108	8 <i>0</i> 2 ⁹	22
620	Correlation and prediction of thermodynamic properties of binary mixtures from perturbed chain statistical associating fluid theory. 2014 , 414, 1-5		2
619	Group-Contribution Method with Proximity Effect for PC-SAFT Molecular Parameters. 2. Application to Association Parameters: Primary Alcohols and Amines. <i>Industrial & amp; Engineering Chemistry Research</i> , 2014 , 53, 909-919	3.9	13
618	Supplementary graphical analysis for the multi-density expansion of associating fluids. 2014 , 31, 374-38	80	
617	Thermodynamic phase behavior of API/polymer solid dispersions. 2014 , 11, 2294-304		102
616	Thermodynamic model for polyelectrolyte hydrogels. 2014 , 118, 10534-42		7
615	Measurement and correlation of vapour pressures of pyridine and thiophene with [EMIM][SCN] ionic liquid. 2014 , 72, 134-138		12
614	Calculation of vaporliquid equilibrium and PVTx properties of geological fluid system with SAFT-LJ EOS including multi-polar contribution. Part III. Extension to waterlight hydrocarbons systems. 2014 , 125, 504-518		14
613	Experimental Measurement and Modeling of Phase Diagrams of Binary Systems Encountered in the Gasoline Desulfurization Process Using Ionic Liquids. <i>Journal of Chemical & Diagrams (Solution Process)</i> 1014, 59, 603-612	2.8	22
613	Gasoline Desulfurization Process Using Ionic Liquids. Journal of Chemical & C	2.8	22
	Gasoline Desulfurization Process Using Ionic Liquids. <i>Journal of Chemical & Data</i> , 2014 , 59, 603-612 Modeling aqueous two-phase systems: II. Inorganic salts and polyether homo- and copolymers as	2.8	
612	Gasoline Desulfurization Process Using Ionic Liquids. <i>Journal of Chemical & Data</i> , 2014, 59, 603-612 Modeling aqueous two-phase systems: II. Inorganic salts and polyether homo- and copolymers as ATPS former. 2014, 375, 306-315 Density gradient theory combined with the PC-SAFT equation of state used for modeling the	2.8	22
612	Gasoline Desulfurization Process Using Ionic Liquids. <i>Journal of Chemical & Data</i> , 2014, 59, 603-612 Modeling aqueous two-phase systems: II. Inorganic salts and polyether homo- and copolymers as ATPS former. 2014, 375, 306-315 Density gradient theory combined with the PC-SAFT equation of state used for modeling the surface tension of associating systems. 2014, 67, 02129	2.8	22
612 611 610	Gasoline Desulfurization Process Using Ionic Liquids. <i>Journal of Chemical & Data</i> , 2014, 59, 603-612 Modeling aqueous two-phase systems: II. Inorganic salts and polyether homo- and copolymers as ATPS former. 2014, 375, 306-315 Density gradient theory combined with the PC-SAFT equation of state used for modeling the surface tension of associating systems. 2014, 67, 02129 Thermodynamics of Polymer Solutions. 2015, 199-246	2.8	22 5

606	Solvent effects on esterification equilibria. AICHE Journal, 2015, 61, 3000-3011	3.6	21
605	Thermodynamic perturbation theory for associating fluids confined in a one-dimensional pore. 2015 , 142, 234906		4
604	The A in SAFT: developing the contribution of association to the Helmholtz free energy within a Wertheim TPT1 treatment of generic Mie fluids. 2015 , 113, 948-984		79
603	Computer-aided molecular design in the continuous-molecular targeting framework using group-contribution PC-SAFT. 2015 , 81, 278-287		82
602	Application of molecular modeling to the vaporliquid equilibrium of alkyl esters (biodiesel) and alcohols systems. 2015 , 161, 34-42		20
601	Vapourllquid equilibrium of propanoic acid + water at 423.2, 453.2 and 483.2 K from 1.87 to 19.38 bar. Experimental and modelling with PR, CPA, PC-SAFT and PCP-SAFT. 2015 , 388, 151-159		9
600	New Variant of the Universal Constants in the Perturbed Chain-Statistical Associating Fluid Theory Equation of State. <i>Industrial & Equation Chemistry Research</i> , 2015 , 54, 1373-1384	3.9	18
599	A Novel Approach for Analyzing the Dissolution Mechanism of Solid Dispersions. 2015 , 32, 2559-78		21
598	Group Contribution Method for Viscosities Based on Entropy Scaling Using the Perturbed-Chain Polar Statistical Associating Fluid Theory. <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 79-60.	42:995	52 ⁷⁸
597	Measurements and equation-of-state modelling of thermodynamic properties of binary mixtures of 1-butyl-1-methylpyrrolidinium tetracyanoborate ionic liquid with molecular compounds. 2015 , 90, 317-3	326	9
596	Thermodynamic Modeling for Efficient Cocrystal Formation. 2015 , 15, 4406-4416		31
595	Solid[Iquid phase equilibria in binary mixtures of functionalized ionic liquids with sugar alcohols: New experimental data and modelling. 2015 , 403, 167-175		11
594	Predicting the Solubility Advantage of Amorphous Pharmaceuticals: A Novel Thermodynamic Approach. 2015 , 12, 2823-33		48
593	Phase equilibria calculation of binary and ternary mixtures of associating fluids applying PC-SAFT equation of state. 2015 , 104, 132-144		12
592	Influence of humidity on the phase behavior of API/polymer formulations. 2015, 94, 352-62		50
591	Solubility and Caloric Properties of Cinnarizine. <i>Journal of Chemical & Data</i> , 2015, 60, 2256-2261	2.8	17
590	A novel approach for predicting the dissolution profiles of pharmaceutical tablets. 2015 , 96, 53-64		8
589	Solving Phase Equilibrium Problems by Means of Avoidance-Based Multiobjectivization. 2015 , 1159-117	71	7

588	Barotropic phenomena in binary mixtures. 2015 , 394, 175-185		9
587	Partition Coefficients of Pharmaceuticals as Functions of Temperature and pH. <i>Industrial & Engineering Chemistry Research</i> , 2015 , 54, 3968-3975	3.9	16
586	Vapourliquid equilibrium at T = 308.15 K for binary systems: Dibromomethane + n-heptane, bromotrichloromethane + n-heptane, bromotrichloromethane + dibromomethane, bromotrichloromethane + bromochloromethane and dibromomethane + bromochloromethane.		3
585	Experimental data and modelling. 2015 , 395, 1-8 Vapor-liquid equilibria of CH4, CO2 and their binary system CH4 + CO2: A comparison between the molecular simulation and equation of state. 2015 , 58, 650-658		4
584	Phase diagrams of binary systems containing tricyanomethanide-based ionic liquids and thiophene or pyridineNew experimental data and PC-SAFT modelling. 2015 , 399, 105-114		19
583	Influence of excipients on solubility and dissolution of pharmaceuticals. 2015, 485, 277-87		32
582	Equation oriented method for Rectisol wash modeling and analysis. 2015, 23, 1530-1535		10
581	Monte Carlo simulation and SAFT modeling study of the solvation thermodynamics of dimethylformamide, dimethylsulfoxide, ethanol and 1-propanol in the ionic liquid trimethylbutylammonium bis(trifluoromethylsulfonyl)imide. 2015 , 17, 7449-62		9
580	Thermodynamic and transport properties of binary mixtures; friction theory coupled with PC-SAFT model. 2015 , 89, 1-6		21
579	Density Functional Theory for Liquid Liquid Interfaces of Mixtures Using the Perturbed-Chain Polar Statistical Associating Fluid Theory Equation of State. <i>Industrial & Discrete Light Research</i> , 2015 , 54, 4633-4642	3.9	28
578	Thermodynamic phase behaviour of indomethacin/PLGA formulations. 2015, 93, 88-94		34
577	Equation-of-state modeling of associating-fluids phase equilibria in nanopores. 2015 , 405, 157-166		35
576	. Industrial & Engineering Chemistry Research, 2015 , 54, 9637-9644	3.9	6
575	Understanding the Thermodynamics of Hydrogen Bonding in Alcohol-Containing Mixtures: Self Association. 2015 , 119, 14086-101		23
574	Transferable Anisotropic United-Atom Force Field Based on the Mie Potential for Phase Equilibrium Calculations: n-Alkanes and n-Olefins. 2015 , 119, 11695-707		38
573	Density and viscosity study of pyridinium based ionic liquids as potential absorbents for natural refrigerants: Experimental and modelling. 2015 , 405, 37-45		13
572	Effect of salts on the solubility of ionic liquids in water: experimental and electrolyte Perturbed-Chain Statistical Associating Fluid Theory. 2015 , 17, 32044-32052		18
571	Thermodynamic study of binary mixtures of 1-butyl-1-methylpyrrolidinium dicyanamide ionic liquid with molecular solvents: new experimental data and modeling with PC-SAFT equation of state. 2015 , 119, 543-51		27

570	Effect of the quadrupolar contribution of CO2 on the vaporllquid equilibria and surface tensions of CO2Bydrocarbon binary mixtures. 2015 , 387, 146-153		8
569	Thermodynamic model for biomass processing in pressure intensified technologies. 2015 , 96, 53-67		16
568	Application of the perturbed chain-SAFT equation of state for modeling CO2 solubility in aqueous monoethanolamine solutions. 2015 , 93, 789-799		12
567	Predicting the Solubility of Pharmaceutical Cocrystals in Solvent/Anti-Solvent Mixtures. 2016 , 21,		18
566	A density functional theory for colloids with two multiple bonding associating sites. 2016 , 28, 244009		13
565	Studies on Thermodynamic and Transport Properties of Binary Mixtures Containing Alcohols and Aniline. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 2510-2515	2.8	20
564	Drug Release Kinetics and Mechanism from PLGA Formulations. AICHE Journal, 2016, 62, 4055-4065	3.6	12
563	Thermodynamic Study of Molecular Interactions in Eutectic Mixtures Containing Camphene. 2016 , 120, 12928-12936		10
562	Phase Equilibria for the Hydroesterification of 10-Undecenoic Acid Methyl Ester. <i>Journal of Chemical & Chemic</i>	2.8	13
561	On the cooperativity of association and reference energy scales in thermodynamic perturbation theory. 2016 , 145, 204104		7
560	High-pressure speed of sound in pure CO 2 and in CO 2 with SO 2 as an impurity using methanol as a doping agent. 2016 , 54, 737-751		9
559	Predicting the Aqueous Solubility of Pharmaceutical Cocrystals As a Function of pH and Temperature. 2016 , 16, 2726-2740		35
558	Influence of Salts on the Partitioning of 5-Hydroxymethylfurfural in Water/MIBK. 2016 , 120, 3797-808		41
557	Influence of electrolytes on liquid-liquid equilibria of water/1-butanol and on the partitioning of 5-hydroxymethylfurfural in water/1-butanol. 2016 , 428, 102-111		28
556	p $\[\]$ Data of (Acetic Acid + Water) at T = (412.6, 443.2, 483.2) K. <i>Journal of Chemical & amp; Engineering Data</i> , 2016 , 61, 2078-2082	2.8	4
555	Modeling and predicting the influence of variable factors on dissolution of crystalline pharmaceuticals. <i>Chemical Engineering Science</i> , 2016 , 145, 10-20	4.4	15
554	Thermophysical and transport properties of binary mixtures containing triethylene glycol and alcohols at different temperatures. 2016 , 124, 399-405		10
553	On the use of molecular-based thermodynamic models to assess the performance of solvents for CO capture processes: monoethanolamine solutions. 2016 , 192, 337-390		9

(2016-2016)

552	Experimental Data and Modeling with Modern Thermodynamic Tools. <i>Industrial & Data & Separation of 2-Phenylethanol From Water by Liquid Liquid Extraction with Ionic Liquids: New Experimental Data and Modeling with Modern Thermodynamic Tools. <i>Industrial & Data & Separation of 2-Phenylethanol From Water by Liquid Liquid Extraction with Ionic Liquids: New Experimental Data and Modeling with Modern Thermodynamic Tools. <i>Industrial & Data & Da</i></i></i>	27
551	An improved thermodynamic model for Wax precipitation using a UNIQUAC + PC-SAFT approach. 2016 , 425, 21-30	23
550	Assessment of thermodynamic models for the design, analysis and optimisation of gas liquefaction systems. 2016 , 183, 43-60	10
549	Prediction of Interfacial Properties of Ternary, Sulfur-containing Mixtures. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 4261-4269	7
548	Modeling of carbon dioxide and water sorption in glassy polymers through PC-SAFT and NET PC-SAFT. 2016 , 104, 149-155	11
547	Interfacial and bulk properties of vapor-liquid equilibria in the system toluene + hydrogen chloride + carbon dioxide by molecular simulation and density gradient theory + PC-SAFT. 2016 , 427, 219-230	28
546	Volumetric and electromagnetic properties of binary mixtures consist of benzene derivatives at different temperature and ternary mixtures with 1,2-dichloroethane at T = 293.15 K with application of the Prigogine lory Patterson theory and PC-SAFT. 2016 , 639, 160-172	2
545	Modeling of activity coefficients of amino acid and electrolyte in aqueous solutions. <i>Journal of Molecular Liquids</i> , 2016 , 223, 1-9	5
544	Interfacial tension and adsorption in the binary system ethanol and carbon dioxide: Experiments, molecular simulation and density gradient theory. 2016 , 427, 476-487	32
543	Inclusion of mPRISM potential for polymer-induced protein interactions enables modeling of second osmotic virial coefficients in aqueous polymer-salt solutions. 2016 , 11, 146-54	7
542	A new equation of state for associating LennardDones fluids with two sites: small bond angle. 2016 , 114, 2548-2557	5
541	Hydrogen Bonding in Polymer Solution. <i>Journal of Chemical & Engineering Data</i> , 2016 , 61, 3438-3442.8	8
540	Thermodynamic Perturbation Theory for Associating Molecules. 2016 , 1-47	3
539	PII measurement and PC-SAFT modeling of N,N-dimethyl formamide, N -methyl formamide, N,N-dimethyl acetamide, and ethylenediamine from $T = (293.15 23.15)$ K and pressures up to 35 MPa. 2016 , 427, 583-593	7
538	Measurement and prediction of phase equilibria of ethylene + vinyl acetate + methanol + poly(ethylene-co-vinyl acetate) systems. 2016 , 429, 98-106	3
537	A modified group-contribution PC-SAFT equation of state for prediction of phase equilibria. 2016 , 430, 33-46	16
536	The NRTL-PRA group contribution EoS for the simultaneous prediction of LLE, VLE and hE of hydrocarbon mixtures with associating compounds. 2016 , 427, 126-142	4
535	Improved estimation of PC-SAFT equation of state parameters using a multi-objective variable-weight cost function. 2016 , 427, 308-319	8

534	Optimization of Production in Reservoirs with Temperature-Dependent Asphaltene Precipitation and Irreversible Flocculation. 2016 ,		О
533	Flash Calculation and Phase Stability Analysis of Reservoir Gas-Water SystemImplication for Extracting Dissolved CH4 by CO2 Injection. 2016 ,		1
532	Thermodynamics of Bioreactions. 2016 , 7, 395-414		36
531	Correlation and prediction of liquid Iquid equilibria for alcohol/hydrocarbon mixtures using PC-SAFT equation of state at high pressure up to 150 MPa. 2016 , 425, 206-214		14
530	Polymorphs, Hydrates, Cocrystals, and Cocrystal Hydrates: Thermodynamic Modeling of Theophylline Systems. 2016 , 16, 4439-4449		26
529	VLE properties of CO2 Based binary systems containing N2, O2 and Ar: Experimental measurements and modelling results with advanced cubic equations of state. 2016 , 428, 18-31		33
528	Predicting the Effect of pH on Stability and Solubility of Polymorphs, Hydrates, and Cocrystals. 2016 , 16, 4136-4147		11
527	Measurement and modelization of VLE of binary mixtures of propyl acetate, butyl acetate or isobutyl acetate with methanol at pressure of 0.6MPa. 2016 , 24, 630-637		3
526	Review and new insights into the application of molecular-based equations of state to water and aqueous solutions. 2016 , 416, 150-173		54
525	Hydrate I f luid phase equilibria modeling using PC-SAFT and Peng R obinson equations of state. 2016 , 413, 209-219		21
524	Thermodynamic properties of a CO2 Irich mixture (CO2+CH3OH) in conditions of interest for carbon dioxide capture and storage technology and other applications. 2016 , 98, 272-281		4
523	Understanding the Thermodynamics of Hydrogen Bonding in Alcohol-Containing Mixtures: Cross-Association. 2016 , 120, 3388-402		34
522	Extensions of the SAFT model for complex association in the bulk and interface. 2016 , 416, 62-71		9
521	A SAFT-VR+DE equation of state based approach for the study of mixed dipolar solvent electrolytes. 2016 , 416, 72-82		10
520	A new equation of state for linear hard chains: Analysis of a third-order expansion of Wertheim's Thermodynamic Perturbation Theory. 2016 , 416, 18-26		8
519	(Solid⊞Iiquid) equilibrium phase diagrams in binary mixtures containing terpenes: New experimental data and analysis of several modelling strategies with modified UNIFAC (Dortmund) and PC-SAFT equation of state. 2016 , 422, 66-77		19
518	Measurement and Modeling of High Pressure Vapor Liquid Equilibrium for Methyl Acetate or Ethyl Acetate with 2-Butanol. Isobaric Data at 1.5 MPa. <i>Journal of Chemical & Data</i> , 2016, 61, 1136-1145	2.8	2
517	PC-SAFT Modeling of CO2 Solubilities in Deep Eutectic Solvents. 2016 , 120, 2300-10		78

516	Density Measurement and Modeling of CO2 B rine System at Temperature and Pressure Corresponding to Storage Conditions. <i>Journal of Chemical & Data</i> , 2016 , 61, 873-880	2.8	5
515	Global phase behaviour in methane plus n-alkanes binary mixtures. 2016 , 111, 151-161		15
514	Linear, cyclic and branched Lennard-Jones chain quartic equation of state templates for associating fluid model development. 2016 , 416, 42-61		
513	Theoretical and experimental study on volumetric and electromagnetic properties of binary systems consisting of 1,2-dichloroethane with benzene and its derivatives at T = (293.15 to 333.15) K. 2016 , 96, 210-221		2
512	Avoiding binary interaction parameters in the GC-PC-SAFT model with a parametrization based in VLE and IDAC data: n-Alkanes and 1-alkanols. 2016 , 412, 9-20		13
511	Estimation of the binary interaction parameter k of the PC-SAFT Equation of State based on pure component parameters using a QSPR method. 2016 , 416, 138-149		11
510	Salt influence on MIBK/water liquid I quid equilibrium: Measuring and modeling with ePC-SAFT and COSMO-RS. 2016 , 416, 83-93		34
509	Phase equilibria of triolein to biodiesel reactor systems. 2016 , 409, 171-192		21
508	Activity coefficients at infinite dilution for different alcohols and ketones in [EMpy][ESO4]: Experimental data and modeling with PC-SAFT. 2016 , 424, 32-40		8
507	PC-SAFT predictions on mixtures of 1-alkyl-3methylimidazolium-bis(trifluroromethanesulphonyl)amide with hydrocarbons, alcohols and aqueous systems using a correlative based binary interaction parameter. 2016 , 59, 69-78		8
506	PC-SAFT predictions of VLE and LLE of systems related to biodiesel production. 2016 , 416, 130-137		25
505	An effect of cation functionalization on thermophysical properties of ionic liquids and solubility of glucose in them IMeasurements and PC-SAFT calculations. 2016 , 92, 81-90		16
504	High pressure viscosity modeling of pure alcohols based on classical and advanced equations of state. 2016 , 58, 57-70		14
503	Novel approach for estimating solubility of solid drugs in supercritical carbon dioxide and critical properties using direct and inverse artificial neural network (ANN). 2017 , 28, 87-99		14
502	Modeling study of the phase behavior of mixtures containing non-ionic glycol ether surfactant. <i>Journal of Molecular Liquids</i> , 2017 , 230, 529-541	6	3
501	Application of the modified Group-Contribution Perturbed-Chain SAFT to branched alkanes, n-olefins and their mixtures. 2017 , 434, 176-192		13
500	Gas Hydrates. 2017 , 405-444		1
499	A density functional theory for association of fluid molecules with a functionalized surface: fluid-wall single and double bonding. 2017 , 29, 044002		6

498	Modeling of interfacial properties of multicomponent systems using density gradient theory and PCP-SAFT. 2017 , 439, 31-42		36
497	Density and Speed of Sound of Binary Mixtures of Ionic Liquid 1-Ethyl-3-methylimidazolium Tetrafluoroborate, N,N-Dimethylformamide, and N,N-Dimethylacetamide at Temperature Range of 293.15B43.15 K: Measurement and PC-SAFT Modeling. <i>Journal of Chemical & Data</i>	2.8	21
496	Evaluation of PR, NRTL, UNIFAC, and PCSAFT on the VLE of Binary Systems Containing Ammonia. <i>Industrial & District Amp; Engineering Chemistry Research</i> , 2017 , 56, 2287-2297	3.9	10
495	Viscosities of Pure Ionic Liquids Using Combinations of Free Volume Theory or Friction Theory with the Cubic, the Cubic Plus Association, and the Perturbed-Chain Statistical Associating Fluid Theory Equations of State at High Pressures. <i>Industrial & Equations of State at High Pressures</i> . <i>Industrial & Equations of State at High Pressures</i> . <i>Industrial & Equations of State at High Pressures</i> .	3.9 2 58	16
494	Thermodynamic models to accurately describe the PVTxy-behavior of water / carbon dioxide mixtures. 2017 , 442, 125-139		27
493	Esterification of fatty acids with supercritical ethanol in a continuous tubular reactor. 2017 , 126, 25-36		18
492	Dimerization of Carboxylic Acids: An Equation of State Approach. 2017, 121, 2153-2163		16
491	Experimental and Computational Study on the Solubility of Argon in Propan-2-ol at High Temperatures. 2017 , 46, 990-991		1
490	Measurement and PC-SAFT modeling of solid-liquid equilibrium of deep eutectic solvents of quaternary ammonium chlorides and carboxylic acids. 2017 , 448, 69-80		66
489	Data Requirements and Modeling for Gas Hydrate-Related Mixtures and a Comparison of Two Association Models. <i>Journal of Chemical & Engineering Data</i> , 2017 , 62, 2592-2605	2.8	11
488	Thermodynamics of enzyme-catalyzed esterifications: I. Succinic acid esterification with ethanol. 2017 , 101, 5973-5984		15
487	A second order thermodynamic perturbation theory for hydrogen bond cooperativity in water. 2017 , 146, 174104		14
486	The Effects of Vehicle Mixtures on Transdermal Absorption: Thermodynamics, Mechanisms, Assessment, and Prediction. 2017 , 95-117		1
485	Predicting solvent effects on the 1-dodecene hydroformylation reaction equilibrium. <i>AICHE Journal</i> , 2017 , 63, 4576-4585	3.6	11
484	Measuring and Predicting Thermodynamic Limitation of an Alcohol Dehydrogenase Reaction. <i>Industrial & Dehydrogenase Reaction Chemistry Research</i> , 2017 , 56, 5535-5546	3.9	11
483	Comparison of predictions of the PC-SAFT equation of state and molecular simulations for the metastable region of binary mixtures. 2017 , 444, 31-36		1
482	Solubility of pharmaceuticals: A comparison between SciPharma, a PC-SAFT-based approach, and NRTL-SAC. 2017 , 226, 913-929		6
481	Studies on thermodynamic properties of butyl acetate/Alkan-2-ol binary mixtures: Measurements and properties modeling. <i>Journal of Molecular Liquids</i> , 2017 , 225, 490-495	6	10

480	Stabilized density gradient theory algorithm for modeling interfacial properties of pure and mixed systems. 2017 , 435, 118-130		23	
479	Impact of the equation of state on calculated adsorption isotherm using DFT. <i>Chemical Engineering Science</i> , 2017 , 171, 513-519	4.4	3	
478	Improving Prediction Accuracy of a Rate-Based Model of an MEA-Based Carbon Capture Process for Large-Scale Commercial Deployment. 2017 , 3, 232-243		9	
477	Modeling of thermophysical behaviour of MCH/Alkan-2-ol binary mixtures. <i>Journal of Molecular Liquids</i> , 2017 , 241, 817-822	6	2	
476	Reaction Equilibrium of the Transamination of (S)-Phenylethylamine: Experiments and ePC-SAFT Modeling. 2017 , 21, 976-986		15	
475	Liquid-liquid equilibrium of hydrogen bonding polymer solutions. 2017 , 121, 1-8		7	
474	Modeling vapor-liquid phase equilibria of methane-water and methane-carbon dioxide-water systems at 274K to 573K and 0.1 to 150IMPa using PRSV equation of state and Wong-Sandler mixing rule. 2017 , 447, 12-26		7	
473	Experimental densities of 2,2,2-trifluoroethanol with 1-butyl-3-methylimidazolium hexafluorophosphate at high pressures and modelling with PC-SAFT. 2017 , 113, 29-40		8	
472	Thermodynamics of mixtures of patchy and spherical colloids of different sizes: A multi-body association theory with complete reference fluid information. 2017 , 146, 164904		7	
471	Prediction of thermodynamic properties of aqueous electrolyte solutions using equation of state. <i>AICHE Journal</i> , 2017 , 63, 5083-5097	3.6	15	
470	PC-SAFT modeling of CO2 solubilities in hydrophobic deep eutectic solvents. 2017 , 448, 94-98		50	
469	Modeling and analysis of dissolution of paracetamol/Eudragit□ formulations. 2017 , 121, 22-31		7	
468	Numerical aspects of classical density functional theory for one-dimensional vapor-liquid interfaces. 2017 , 444, 1-12		25	
467	Thermodynamic Modeling with Equations of State: Present Challenges with Established Methods. <i>Industrial & Engineering Chemistry Research</i> , 2017 , 56, 3503-3515	3.9	56	
466	The phase and interfacial properties of azeotropic refrigerants: the prediction of aneotropes from molecular theory. 2017 , 19, 8977-8988		26	
465	Classical Density Functional Theory for Liquid E luid Interfaces and Confined Systems: A Functional for the Perturbed-Chain Polar Statistical Associating Fluid Theory Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2017 , 56, 4119-4135	3.9	62	
464	Performance of a vapour absorption heat transformer operating with ionic liquids and ammonia. 2017 , 141, 924-936		17	
463	Thermodynamics of enzyme-catalyzed esterifications: II. Levulinic acid esterification with short-chain alcohols. 2017 , 101, 7509-7521		20	

462	Isothermal Vaporliquid Equilibria for Binary Mixtures of Methyl Nonafluorobutyl Ether + Acetone, Cyclopentyl Methyl Ether, Ethyl Acetate, n-Heptane, Methanol, and Toluene. <i>Journal of Chemical & Camp; Engineering Data</i> , 2017 , 62, 3878-3888	2.8	12
461	Vapourliquid interfacial properties of n-alkanes. <i>Journal of Molecular Liquids</i> , 2017 , 248, 253-263	5	2
460	Impact of Polymer Type and Relative Humidity on the Long-Term Physical Stability of Amorphous Solid Dispersions. 2017 , 14, 4374-4386		57
459	Prediction of water content of natural gases using the PC-SAFT equation of state. 2017 , 453, 40-45		3
458	Measurements and Modeling of VLE Data for Butyl Acetate with 2-Propanol or 2-Butanol. Binary Systems at 0.15 and 0.6 MPa. <i>Journal of Chemical & Engineering Data</i> , 2017 , 62, 2296-2306	2.8	6
457	Influence of Temperature and Carbon Chain on Thermophysical Properties of Benzaldehyde/Alkan-2-ol Binary Mixtures. <i>Journal of Chemical & Data, Engineering Data</i> , 2017 , 62, 2406-24	28 112	3
456	CO2 + n-dodecane + 3,7-dimethyl-1-octanol: High pressure experimental phase equilibria data and thermodynamic modelling. 2017 , 130, 105-117		4
455	Predicting the Solubility of CO2 in Toluene + Ionic Liquid Mixtures with PC-SAFT. <i>Industrial & Engineering Chemistry Research</i> , 2017 , 56, 9885-9894	3.9	12
454	Quasi-Chemical PC-SAFT: An Extended Perturbed Chain-Statistical Associating Fluid Theory for Lattice-Fluid Mixtures. 2017 , 121, 8338-8347		3
453	Phase Diagrams in Representative Terpenoid Systems: Measurements and Calculations with Leading Thermodynamic Models. <i>Industrial & Engineering Chemistry Research</i> , 2017 , 56, 9753-9761	3.9	6
452	Measurement and Modeling the Excess Molar Volumes and Refractive Index Deviations of Binary Mixtures of 2-Propanol, 2-Butanol and 2-Pentanol with N-Propylamine. 2017 , 46, 2135-2158		10
45 ¹	Perturbation theory for water with an associating reference fluid. 2017 , 96, 052602		10
450	Thermodynamic properties and CO 2 solubility of monoethanolamine mixtures: Experimental measurements and thermodynamic modeling. 2017 , 449, 175-185		8
449	Phase Behavior of Binary Mixtures Containing Succinic Acid or Its Esters. <i>Journal of Chemical & Engineering Data</i> , 2017 , 62, 1983-1993	2.8	9
448	The polyazeotropic behaviour of the benzene plus hexafluorobenzene system revisited. 2017 , 113, 340-3	349	7
447	Thermophysical properties of oxygenated thiophene derivatives: Experimental data and modelling. 2017 , 113, 330-339		6
446	Studies on physicochemical behavior of binary mixtures containing propanal and Alkan-2-ol. 2017 , 113, 315-320		7
445	Solubility of carbon monoxide in bio-oil compounds. 2017 , 105, 296-311		4

444	Modelling of phase equilibrium of natural gas mixtures containing associating compounds. 2017 , 433, 135-148		12
443	Phase equilibrium of CCS mixtures: Equation of state modeling and Monte Carlo simulation. 2017 , 119, 169-202		23
442	Long-Term Physical Stability of PVP- and PVPVA-Amorphous Solid Dispersions. 2017 , 14, 157-171		71
441	Prediction of vapor-liquid and liquid-liquid equilibria at high pressures of 2-alkoxyethanol mixtures using PC-SAFT EoS. 2017 , 434, 7-20		13
440	Measuring and Predicting the Extraction Behavior of Biogenic Formic Acid in Biphasic Aqueous/Organic Reaction Mixtures. 2017 , 2, 8982-8989		8
439	Evaluation of Thermodynamic Models for Predicting Phase Equilibria of (hbox {CO}_{2}) + Impurity Binary Mixture. 2018 , 39, 1		7
438	Pure Substance and Mixture Viscosities Based on Entropy Scaling and an Analytic Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 4095-4114	3.9	45
437	Mixture Equation of State for Water with an Associating Reference Fluid. <i>Industrial & amp;</i> Engineering Chemistry Research, 2018 , 57, 4070-4080	3.9	8
436	Light-scattering data of protein and polymer solutions: A new approach for model validation and parameter estimation. 2018 , 465, 65-72		5
435	Solubility of carbon dioxide in methanol from 213.15 K to 273.15 K: Measurement and modeling. 2018 , 471, 40-54		4
434	Extensive Study of the Capabilities and Limitations of the CPA and sPC-SAFT Equations of State in Modeling a Wide Range of Acetic Acid Properties. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 5690-5704	3.9	10
433	Modeling of the phase behavior of CO 2 in water, methanol, ethanol and acetone by different equations of state. 2018 , 469, 9-25		2
432	Modified Density Gradient Theory for Surfactant Molecules Applied to Oil/Water Interfaces. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 7643-7654	3.9	14
431	Mutual Influence of Furfural and Furancarboxylic Acids on Their Solubility in Aqueous Solutions: Experiments and Perturbed-Chain Statistical Associating Fluid Theory (PC-SAFT) Predictions. <i>Journal of Chemical & Data</i> , 2018, 63, 1460-1470	2.8	10
430	Pervaporation performance of crosslinked PVA membranes in the vicinity of the glass transition temperature. 2018 , 553, 63-69		31
429	Vapor - liquid equilibrium of the carbon dioxide/methane mixture at three isotherms. 2018 , 462, 44-58		9
428	Solubility on tetrahydrofurfuryl acrylate effect for the poly[tetrahydrofurfuryl acrylate] in supercritical carbon dioxide and dimethyl ether. 2018 , 135, 211-217		6
427	Phase behavior for the 2-(trimethylsilyloxy)ethyl methacrylate and 3-(trimethoxysilyl)propyl methacrylate in supercritical carbon dioxide. 2018 , 462, 1-5		4

426	Modeling of physical properties and vapor liquid equilibrium of ethylene and ethylene mixtures with equations of state. 2018 , 470, 149-163		15
425	A Comparative Study of the Perturbed-Chain Statistical Associating Fluid Theory Equation of State and Activity Coefficient Models in Phase Equilibria Calculations for Mixtures Containing Associating and Polar Components. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 3014-3030	3.9	10
424	Viscosity Modeling of Ionic Liquids Using the Friction Theory and a Simple Cubic Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 1109-1120	3.9	5
423	Physical stability of API/polymer-blend amorphous solid dispersions. 2018 , 124, 147-157		39
422	CO2 + 3,7-dimethyl-1-octanol + 1-decanol: High pressure experimental phase equilibria data and thermodynamic modelling. 2018 , 136, 82-94		2
421	Renewable platform chemicals: Thermochemical study of levulinic acid esters. 2018 , 659, 213-221		19
420	Phase equilibrium of PVAcI+ICO2 binary systems and PVAcI+ICO2I+Iethanol ternary systems. 2018 , 458, 264-271		9
419	Phase Behavior for Poly(vinylacetate) + Carbon Dioxide + Cosolvent Ternary Systems. <i>Journal of Chemical & Che</i>	2.8	8
418	Mutual Impact of Phase Separation/Crystallization and Water Sorption in Amorphous Solid Dispersions. 2018 , 15, 669-678		17
417	Thermodynamic Modeling and Simulation of Biodiesel Systems at Supercritical Conditions. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 751-767	3.9	8
416	Modeling Thermodynamic Properties of Isomeric Alkanes with a New Branched Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 1679-1688	3.9	3
415	Molecular Models for the Hydrogen Age: Hydrogen, Nitrogen, Oxygen, Argon, and Water. <i>Journal of Chemical & Ch</i>	2.8	13
414	A viscosity model for ionic liquids based on the Eyring's theory and a cubic EoS. <i>Journal of Molecular Liquids</i> , 2018 , 262, 161-174	6	8
413	A general mixture equation of state for double bonding carboxylic acids with 2 association sites. 2018 , 148, 174103		3
412	Physical Stability of Amorphous Solid Dispersions: a Physicochemical Perspective with Thermodynamic, Kinetic and Environmental Aspects. 2018 , 35, 125		52
411	Measurement and prediction of phase equilibria of ethylene + methyl acrylate + poly(ethylene-co-methyl acrylate) systems. 2018 , 465, 100-106		1
410	Phase behavior of tetrahydrofurfuryl methacrylate and poly(tetrahydrofurfuryl methacrylate) in supercritical carbon dioxide. 2018 , 25, 39-45		11
409	Thermodynamic Modeling of Multicomponent Liquid Liquid Equilibria in Ionic Liquid Systems with PC-SAFT Equation of State. <i>Industrial & amp; Engineering Chemistry Research</i> , 2018 , 57, 5413-5432	3.9	4

408	Guaiacol and its mixtures: New data and predictive models part 1: Phase equilibrium. 2018, 470, 75-90		4
407	Comparison of performance of a vapor absorption refrigeration system operating with some hydrofluorocarbons and hydrofluoroolefins as refrigerants along with ionic liquid [hmim][TF2N] as the absorbent. 2018 , 88, 370-382		28
406	Multi-criteria optimization for parameterization of SAFT-type equations of state for water. <i>AICHE Journal</i> , 2018 , 64, 226-237	3.6	24
405	Integrated solvent and process design for continuous crystallization and solvent recycling using PC-SAFT. <i>AICHE Journal</i> , 2018 , 64, 1205-1216	3.6	14
404	A general viscosity model for deep eutectic solvents: The free volume theory coupled with association equations of state. 2018 , 470, 193-202		55
403	Phase behavior of Carbon dioxide/Trimethoxy(methyl)silane and Methylsilicate 51 system. 2018 , 455, 6-14		8
402	Predicting the thermodynamic properties of experimental mixed-solvent electrolyte systems using the SAFT-VR+DE equation of state. 2018 , 460, 105-118		9
401	Modelling the thermodynamics of air-component mixtures (N2, O2 and Ar): Comparison and performance analysis of available models. 2018 , 458, 278-287		2
400	Modeling properties of the one-dimensional vapor-liquid interface: Application of classical density functional and density gradient theory. 2018 , 458, 243-252		22
399	Thermodynamic prediction of the solvent effect on a transesterification reaction. <i>Chemical Engineering Science</i> , 2018 , 176, 264-269	4.4	8
398	Investigating phase separation in amorphous solid dispersions via Raman mapping. 2018 , 535, 245-252		25
397	Modeling binary mixtures of n-alkanes and water using PC-SAFT. 2018 , 470, 203-211		25
396	Phase behaviors for the poly(2-phenylethyl methacrylate) in supercritical fluid solvents: Experiment and PC-SAFT EoS. 2018 , 59, 403-409		9
395	CO2 solubility in small carboxylic acids: Monte Carlo simulations and PC-SAFT modeling. 2018 , 458, 1-8		7
394	The friction theory for modeling the viscosities of deep eutectic solvents using the CPA and PC-SAFT equations of state. <i>Journal of Molecular Liquids</i> , 2018 , 249, 554-561	6	28
393	. 2018,		2
			_
392	Thermodynamic Modeling of Natural Gas and Gas Condensate Mixtures. 2018, 57-88		

390	Some Observations Regarding the Association Kernel of SAFT-VR-Mie. Is the Molecularly Inspired Contribution Always Necessary?. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 15869-15883 ³⁻⁹)	5
389	Choosing Appropriate Solvents for ASD Preparation. 2018 , 15, 5397-5409		13
388	Effect of specific interaction of CO2 with poly(ethylene glycol) on phase behavior. 2018, 28, 228-234		4
387	Modeling of the Mixture Critical Locus with a Modified Cubic Plus Association (CPA) EoS: Aromatics, Ketones, Ethers, Diethyl Carbonate, and THF. <i>Industrial & Engineering Chemistry Research</i> , 2018 3.9, 57, 15857-15868)	5
386	Process Modeling, Simulation and Optimization: From Single Solutions to a Multitude of Solutions to Support Decision Making. 2018 , 90, 1727-1738		12
385	Investigation of Molecular Interactions in Binary Mixtures of n-Butyl Acetate and (C6 🖸 10) 1-Alkanol: PC-SAFT Model. <i>Journal of Chemical & Data, 2018, 63, 3881-3888</i>	3	26
384	Tunable Hydrophobic Eutectic Solvents Based on Terpenes and Monocarboxylic Acids. 2018 , 6, 8836-8846		133
383	A classical density functional theory for vapor-liquid interfaces consistent with the heterosegmented group-contribution perturbed-chain polar statistical associating fluid theory. 2018 , 472, 117-127		10
382	Correlation Studies of Cyclohexanone/(C5I10) Alkan-1-ol Binary Mixtures: PC-SAFT Model and Free Volume Theory. <i>Journal of Chemical & Data</i> , 2018 , 63, 2257-2265	}	11
381	Accurate modeling of multiphase behavior of aqueous systems. I. Alkanes, alkenes, cycloalkanes, alcohols, aromatics. 2018 , 473, 201-219		15
380	Comparison of two modelling approaches for the interfacial tension of binary aqueous mixtures. <i>Journal of Molecular Liquids</i> , 2018 , 266, 309-320		13
379	Prediction of Gas and Liquid Solubility in Organic Polymers Based on the PR+COSMOSAC Equation of State. <i>Industrial & Discourse amp; Engineering Chemistry Research</i> , 2018 , 57, 10628-10639)	6
378	A molecular equation of state for alcohols which includes steric hindrance in hydrogen bonding. 2018 , 149, 044505		О
377	Computer-Aided Molecular Design: Fundamentals, Methods, and Applications. 2018,		14
376	The Role of Polyfunctionality in the Formation of [Ch]Cl-Carboxylic Acid-Based Deep Eutectic Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 11195-11209)	34
375	Modeling of the Mixture Critical Locus with a Modified Cubic Plus Association Equation of State: Water, Alkanols, Amines, and Alkanes. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 10649-ੴ	662	7
374	Predictive Model for Pressure Volume Temperature Properties and Asphaltene Instability of Crude Oils under Gas Injection. <i>Energy & Damp; Fuels</i> , 2018 , 32, 8318-8328	[8
373	Vapor-liquid and liquid-liquid equilibrium modeling of systems involving ethanol, water, and ethyl valerate (valeric acid) using the PC-SAFT equation of state. 2018 , 474, 92-99		1

372	Measuring and modeling thermodynamic properties of aqueous lysozyme and BSA solutions. 2018 , 472, 62-74		10
371	Computation of partial molar properties using continuous fractional component Monte Carlo. 2018 , 116, 3331-3344		19
370	Using a Volume Shift in Perturbed-Chain Statistical Associating Fluid Theory To Improve the Description of Speed of Sound and Other Derivative Properties. <i>Industrial & Description of Speed of Sound and Other Derivative Properties and Statistical & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. <i>Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. <i>Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. <i>Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. <i>Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed of Sound and Other Derivative Properties. Industrial & Description of Speed </i></i></i></i></i>	.9	9
369	Comprehensive Residual Oil Hydrocracking Reaction Kinetic Modeling Combined with Effective Phase Equilibrium Calculation. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 11271-11279 ³	.9	2
368	Identifying Pure-Component Parameters of an Analytic Equation of State Using Experimental Surface Tension or Molecular Simulations with a Transferable Force Field. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 12254-12263	.9	3
367	Modeling phase behavior of poly(lactic acid) in supercritical fluids. 2018 , 147, 164-169		3
366	Measurement and Modelization of VLE for Butyl Acetate with Methanol, Ethanol, 1-Propanol, and 1-Butanol. Experimental Data at 0.15 MPa. <i>Journal of Chemical & Chemic</i>	242	3
365	Influence of Liquid Structure on Fickian Diffusion in Binary Mixtures of n-Hexane and Carbon Dioxide Probed by Dynamic Light Scattering, Raman Spectroscopy, and Molecular Dynamics Simulations. 2018 , 122, 7122-7133		25
364	Global phase behaviour in carbon dioxide plus n-alkanes binary mixtures. 2018 , 140, 147-158		5
363	Predicting the Phase Behavior of Alcohols, Aromatic Alcohols, and Their Mixtures Using the Modified Group-Contribution Perturbed-Chain Statistical Associating Fluid Theory. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 16963-16977	.9	8
362	Loss of Methanol and Monoethylene Glycol in VLE and LLE: Prediction of Hydrate Inhibitor Partition. <i>Journal of Chemical & Data</i> , 2019 , 64, 3889-3903	8	2
361	Nucleation rates of water using Adjusted SAFT-0 EOS. 2019 , 501, 112272		O
360	Modeling of Gas Solubility Using the Electrolyte Cubic Plus Association Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 17555-17567	.9	15
359	Density variations of TMAO solutions in the kilobar range: Experiments, PC-SAFT predictions, and molecular dynamics simulations. 2019 , 253, 106222		7
358	Prediction of asphaltene precipitation upon injection of various gases at near-wellbore conditions: A simulation study using PC-SAFT EoS. 2019 , 74, 63		5
357	Thermodynamic data for cryogenic carbon dioxide capture from natural gas: A review. 2019 , 102, 85-104		30
356	Comparison of SAFT-VR-Mie and CP-PC-SAFT in predicting phase behavior of associating systems IV. MethanolBliphatic hydrocarbons. <i>Journal of Molecular Liquids</i> , 2019 , 291, 111321	í	7
355	A doubly associated reference perturbation theory for water. 2019 , 500, 112252		4

354	Modeling Binary Mixtures of Water + Light Hydrocarbon Using the Perturbed-Chain Statistical Associating Fluid Theory with Induced Association: Improvement in Describing All Equilibrium Phases. 2019 , 3, 2569-2581		О
353	Solubility of pharmaceutical ingredients in triglycerides. 2019 , 145, 113-120		10
352	Vapor Pressures, Densities, and PC-SAFT Parameters for 11 Bio-compounds. 2019 , 40, 1		19
351	Measurement and Modeling of Lactose Solubility in Aqueous Electrolyte Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 20797-20805	3.9	7
350	Second-Order Differential Accelerators Based on the Geometry of Equilibrium for Thermodynamic Calculations. Part I. Pure Fluids. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 20838-20846	3.9	2
349	(IVE, T) Measurements of the Ternary Mixture (Dibutyl Ether + 1-Heptanol + Heptane) at Temperatures up to 393.15 K and Pressures up to 140 MPa and Modeling Using the Peng R obinson and PC-SAFT Equations of State. <i>Journal of Chemical & Discourse Engineering Data</i> , 2019 , 64, 3861-3873	2.8	9
348	THERMODYNAMIC ANALYSIS AND MODELING OF BRAZILIAN CRUDE OIL AND ASPHALTENE SYSTEMS: AN EXPERIMENTAL MEASUREMENT AND A PC-SAFT APPLICATION. 2019 , 36, 557-571		3
347	High-Pressure Soybean Oil Biodiesel Density: Experimental Measurements, Correlation by Tait Equation, and Perturbed Chain SAFT (PC-SAFT) Modeling. <i>Journal of Chemical & Chemic</i>	2.8	11
346	Structure and thermodynamics of aqueous urea solutions from ambient to kilobar pressures: From thermodynamic modeling, experiments, and first principles simulations to an accurate force field description. 2019 , 254, 106260		7
345	Thermodynamic Properties of 1-Hexyl-3-methylimidazolium Nitrate and 1-Alkanols Mixtures: PC-SAFT Model. <i>Journal of Chemical & Engineering Data</i> , 2019 , 64, 4465-4473	2.8	18
344	Modeling H2S solubility in aqueous N-methyldiethanolamine solution using a new ePC_SAFT-MB equation of state. 2019 , 502, 112289		3
343	Thermodynamic modeling of ternary systems containing imidazolium-based ionic liquids and acid gases using SRK, Peng-Robinson, CPA and PC-SAFT equations of state. 2019 , 37, 2420-2428		1
342	Recycling a carbon fibre reinforced polymer with a supercritical acetone/water solvent mixture: Comprehensive analysis of reaction kinetics. 2019 , 161, 225-234		9
341	Comparison of SAFT-VR-Mie and CP-PC-SAFT in predicting phase behavior of associating systems III. Aliphatic hydrocarbons - 1-propanol, 1-butanol and 1-pentanol. <i>Journal of Molecular Liquids</i> , 2019 , 279, 492-502	6	9
340	Experimental Data of Fluid Phase Equilibria- Correlation and Prediction Models: A Review. 2019 , 7, 277		12
339	Vapor Liquid Equilibria of 1-Ethyl-3-methylimidazolium Triflate (CmimTfO) and -Alkyl Alcohol Mixtures. 2019 , 123, 6076-6089		6
338	Molecular modeling of the solubility of low global warming potential refrigerants in polyol ester lubricants. 2019 , 103, 145-154		12
337	Theoretical and experimental study of physicochemical behavior of binary mixtures: SAFT and PC-SAFT models. 2019 , 131, 1		3

336	Modeling of Gas Solubility in Hydrocarbons Using the Perturbed-Chain Statistical Associating Fluid Theory Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 12347-12360	3.9	6
335	A PC-SAFT model for hydrocarbons IV: Water-hydrocarbon phase behavior including petroleum pseudo-components. 2019 , 497, 79-86		8
334	Group contribution-based property estimation methods: advances and perspectives. 2019 , 23, 184-196		34
333	Phase Behavior Modeling of Mixtures Containing N-, S-, and O-Heterocyclic Compounds Using PC-SAFT Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 11038-11059	3.9	8
332	Bond cooperativity and ring formation in hydrogen fluoride thermodynamic properties: A two-density formalism framework. 2019 , 150, 174503		4
331	Characterization and determination of thermodynamic properties of waste cooking oil biodiesel: Experimental, correlation and modeling density over a wide temperature range up to 393.15 and pressure up to 140 MPa. 2019 , 497, 87-96		9
330	CO2 + n-dodecane + 1-decanol: High pressure experimental phase equilibria data and thermodynamic modelling. 2019 , 151, 49-62		1
329	Thermodynamic Approach for Co-crystal Screening. 2019 , 19, 3253-3264		13
328	Heterosegmental Modeling of Long-Chain Molecules and Related Mixtures Using PC-SAFT: 2. Associating Compounds. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 4625-4643	3.9	6
327	Application of the Perturbed-Chain SAFT to Phase Equilibria in the Fischer Tropsch Synthesis. <i>Industrial & Discourse Chemistry Research</i> , 2019 , 58, 8387-8400	3.9	6
326	Density and Volumetric Properties of Binary Mixtures of CO2 + Hexadecane from (303.2 to 473.2) K and Pressures up to 50.0 MPa. <i>Journal of Chemical & Engineering Data</i> , 2019 , 64, 2568-2577	2.8	2
325	A GENERAL FRAMEWORK FOR SOLID I IQUID EQUILIBRIA IN PHARMACEUTICAL SYSTEMS. 2019 , 439-46	6	
324	Activity-based analysis of potentiometric pH titrations. 2019 , 1075, 49-56		1
323	Using Volume Shifts To Improve the Description of Speed of Sound and Other Derivative Properties with Cubic Equations of State. <i>Industrial & Engineering Chemistry Research</i> , 2019 ,	3.9	2
322	New phase equilibrium data at ambient and high pressure for strongly asymmetric mixtures containing menthol. <i>Journal of Molecular Liquids</i> , 2019 , 286, 110819	6	1
321	Application of the Modified Group Contribution PC-SAFT to Carboxylic Acids and Their Mixtures. <i>Industrial & Damp; Engineering Chemistry Research</i> , 2019 ,	3.9	7
320	Surrogate modeling of phase equilibrium calculations using adaptive sampling. 2019 , 126, 204-217		17
319	Incorporating a concentration-dependent dielectric constant into ePC-SAFT. An application to binary mixtures containing ionic liquids. 2019 , 492, 26-33		29

318	Thermodynamic Modeling of Triglycerides using PC-SAFT. <i>Journal of Chemical & Data</i> , 2019 , 64, 1446-1453	2.8	10
317	Observations regarding the first and second order thermodynamic derivative properties of non-polar and light polar fluids by perturbed chain-SAFT equations of state. 2019 , 99, 78-86		1
316	Reply to Comment on P erturbed-Chain SAFT: An Equation of State Based on a Perturbation Theory for Chain Molecules [Industrial & amp; Engineering Chemistry Research, 2019 , 58, 5744-5745	3.9	6
315	Thermodynamic Properties of Systems Comprising Esters: Experimental Data and Modeling with PC-SAFT and SAFT-IMie. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 6841-6849	3.9	5
314	Density of biofuel mixtures (Dibutyl ether Heptane) at temperatures from (298.15B93.15) K and at pressures up to 140IMPa: Experimental data and PC-SAFT modeling. 2019 , 491, 35-44		12
313	Application of SAFT-VRE in the Flowsheet Simulation of an Advanced PUREX Process. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 3822-3831	3.9	4
312	110th Anniversary: Distribution Coefficients of Furfural and 5-Hydroxymethylfurfural in Hydrophobic Deep Eutectic Solvent + Water Systems: Experiments and Perturbed-Chain Statistical Associating Fluid Theory Predictions. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 4240-426	3.9 47	31
311	Evaluation of PC-SAFT on the Saturation Pressure Prediction of Different Mixture System at High Temperatures and Pressures. 2019 , 585, 012088		
310	Design of Extractive Reaction Systems. 2019 , 91, 1766-1776		3
309	Liquid Diquid Equilibria for Separation of Alcohols from Esters Using Deep Eutectic Solvents Based on Choline Chloride: Experimental Study and Thermodynamic Modeling. <i>Journal of Chemical & Engineering Data</i> , 2019 , 64, 6049-6059	2.8	9
308	Free-volume theory coupled with modified group-contribution PC-SAFT for predicting the viscosities. II. Alcohols and their mixtures. 2019 , 502, 112298		1
307	Thermodynamic modelling of wax precipitation using PC-SAFT in a multi-solid framework. 2019 , 21, 229		4
306	Thermodynamic analysis of biodiesel production systems at supercritical conditions. 2019 , 484, 106-113		7
305	Modeling phase behavior of Poly(e-caprolactone) solutions at high pressure. 2019 , 483, 116-121		3
304	Experimental density and PC-SAFT modeling of biofuel mixtures (DBE + 1-Heptanol) at temperatures from (298.15 to 393.15) K and at pressures up to 140 MPa. 2019 , 131, 269-285		11
303	Modelling of planar and spherical phase interfaces for multicomponent systems using density gradient theory. 2019 , 483, 70-83		2
302	Modeling the phase behavior of refrigerants with ionic liquids using the QC-PC-SAFT equation of state. <i>Journal of Molecular Liquids</i> , 2019 , 274, 497-504	6	8
301	Phase Behavior of Natural Gas Systems. 2019 , 37-101		1

300 Liquid Liquid Liquid Liquid Liquid Liquid Equilibrium in Food Processes. **2019**, 275-334

299	Modeling the phase equilibria of asymmetric hydrocarbon mixtures using molecular simulation and equations of state. <i>AICHE Journal</i> , 2019 , 65, 792-803	3.6	10
298	Heterosegmental Modeling of Long-Chain Molecules and Related Mixtures using PC-SAFT: 1. Polar Compounds. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 2551-2574	3.9	9
297	Thermophysical properties of 1-Hexyl-3-methylimidazolium nitrate and 2-alkanol; measurement and modeling. 2020 , 503, 112324		9
296	Comparison between a soft computing model and thermodynamic models for prediction of phase equilibria in binary mixtures containing 1-alkanol, n-alkane, and CO2. 2020 , 503, 112307		2
295	Henry Law Constant of Noble Gases in Water, Methanol, Ethanol, and Isopropanol by Experiment and Molecular Simulation. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 1180-1188	2.8	3
294	Guide to efficient solution of PC-SAFT classical Density Functional Theory in various Coordinate Systems using fast Fourier and similar Transforms. 2020 , 504, 112306		18
293	Thermodynamic analysis, experimental and kinetic modeling of levulinic acid esterification with ethanol at supercritical conditions. 2020 , 260, 116376		11
292	Prediction of vapor pressure and density for nonaqueous solutions of the ionic liquid 1-ethyl-3-methylimidazolium ethyl sulfate using PC-SAFT equation of state. 2020 , 506, 112320		4
291	Implementation and Application of Model-Based Design of Experiments in a Flowsheet Simulator. Journal of Chemical & Design Data, 2020, 65, 1135-1145	2.8	10
2 90	Ternary System CO2/2-MTHF/Water E xperimental Study and Thermodynamic Modeling. <i>Journal of Chemical & Chemica</i>	2.8	4
289	Modeling of Interfacial Tensions of Long-Chain Molecules and Related Mixtures Using Perturbed Chain-Statistical Associating Fluid Theory and the Density Gradient Theory. <i>Journal of Chemical & Chemical Regineering Data</i> , 2020 , 65, 1005-1018	2.8	5
288	Competitive H2S ICO2 absorption in reactive aqueous methyldiethanolamine solution: Prediction with ePC-SAFT. 2020 , 511, 112453		11
287	Asphaltene phase diagram prediction using PC-SAFT EOS: Development of a new robust algorithm for VLLE calculations. <i>Journal of Molecular Liquids</i> , 2020 , 300, 112328	6	1
286	A method for thermodynamic modeling of H2S solubility using PC-SAFT equation of state based on a ternary solution of water, methyldiethanolamine and hydrogen sulfide. <i>Journal of Molecular Liquids</i> , 2020 , 299, 112113	6	6
285	Correctly Measuring and Predicting Solubilities of Solvates, Hydrates, and Polymorphs. 2020 , 20, 723-73	35	14
284	Phase equilibria of systems containing oxygenated compounds: Polar or ₿seudo-association□ approach?. 2020 , 508, 112435		6
283	Experimental solubility and density studies on aqueous solutions of quaternary ammonium halides, and thermodynamic modelling for melting enthalpy estimations. <i>Journal of Molecular Liquids</i> , 2020 , 300, 112281	6	6

282	Recent advances of pharmaceutical crystallization theories. 2020 , 28, 935-948		9
281	A PC-SAFT model for hydrocarbons V: Alcohol-hydrocarbon phase behavior with application to petroleum pseudo-components. 2020 , 507, 112420		6
280	Experimental and modeling study of diisopropyl ether and 2-alkanol; PC-SAFT model and free volume theory. 2020 , 142, 106025		15
279	A Thermodynamic Approach for Simultaneous Solvent and Process Design of Continuous Reactive Crystallization with Recycling. 2020 , 48, 805-810		1
278	Molecular dynamic simulation and SAFT modeling of the viscosity and self-diffusion coefficient of low global warming potential refrigerants. <i>Journal of Molecular Liquids</i> , 2020 , 317, 113998	6	6
277	Rapid identification of tailor-made aqueous two-phase systems for the extractive purification of high-value biomolecules. <i>Journal of Molecular Liquids</i> , 2020 , 314, 113655	6	7
276	Mixture Solubility Parameters from Experimental Data and Perturbed-Chain Statistical Associating Fluid Theory. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 5801-5808	2.8	
275	Investigating Various Parametrization Strategies for Pharmaceuticals within the PC-SAFT Equation of State. <i>Journal of Chemical & Data</i> , 2020, 65, 5753-5767	2.8	6
274	Bulk and Interfacial Properties of the Decane + Water System in the Presence of Methane, Carbon Dioxide, and Their Mixture. 2020 , 124, 9556-9569		15
273	Physical stability of hydroxypropyl methylcellulose-based amorphous solid dispersions: Experimental and computational study. 2020 , 589, 119845		12
272	Experimental determination and thermodynamic modeling of clathrate hydrate stability conditions in methane + hydrogen sulfide + water system. 2020 , 83, 103549		3
271	Density and Viscosity of CO2 + Ethanol Binary Systems Measured by a Capillary Viscometer from 308.15 to 338.15 K and 15 to 45 MPa. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 3820-3833	2.8	4
270	Thermodynamic study of binary mixture of 2-butanol + monoethanolamine at different temperatures; PC-SAFT and ERAS models. <i>Journal of Molecular Liquids</i> , 2020 , 320, 114461	6	2
269	Evaluating the Performance of the PC-SAFT and CPA Equations of State on Anomalous Properties of Water. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 5718-5734	2.8	6
268	SEPP: Segment-Based Equation of State Parameter Prediction. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 5830-5843	2.8	2
267	Beyond Wertheim Multi-density Theory: Steric Hindrance and Associated Rings in a Two-Density Formalism for Binary Mixtures of Molecules with Two Associating Sites. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 5743-5752	2.8	2
266	Promising Thiolanium Ionic Liquid for Extraction of Aromatics from Aliphatics: Experiments and Modeling. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 15707-15717	3.9	7
265	On the study of the vapor-liquid interface of associating fluids with classical density functional theory. 2020 , 522, 112744		3

264	Review and comparison of equations of state for the Lennard-Jones fluid. 2020 , 523, 112772		14
263	Molecular modelling techniques for predicting liquid-liquid interfacial properties of methanol plus alkane (-hexane, -heptane, -octane) mixtures. 2020 , 22, 27121-27133		O
262	Application of ePC_SAFT-MB EoS in prediction of VLE for CO2+MDEA+H2O ternary and H2O+MDEA+CO2-CH4 quaternary mixtures. 2020 , 525, 112801		1
261	Characteristic Curves of the Lennard-Jones Fluid. 2020 , 41, 147		5
260	In-Silico Screening of Lipid-Based Drug Delivery Systems. 2020 , 37, 249		2
259	Non-invasive, spatially averaged temperature measurements of falling acetone droplets in nitrogen atmosphere at elevated pressures and temperatures. 2020 , 166, 105025		5
258	Estimation of Thermodynamic Properties and Phase Equilibria in Systems of Deep Eutectic Solvents by PC-SAFT EoS. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 22292-22300	3.9	8
257	Vaporlliquid Equilibrium of Ionic Liquid 7-Methyl-1,5,7-triazabicyclo[4.4.0]dec-5-enium Acetate and Its Mixtures with Water. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 2405-2421	2.8	7
256	Solubility of Pharmaceutical Ingredients in Natural Edible Oils. 2020 , 17, 2499-2507		9
255	5-Hydroxymethylfurfural Synthesis in Nonaqueous Two-Phase Systems (NTPS) B C-SAFT Predictions and Validation. 2020 , 24, 1052-1062		6
254	Vapor-liquid equilibrium calculations at specified composition, density and temperature with the perturbed chain statistical associating fluid theory (PC-SAFT) equation of state. 2020 , 521, 112661		2
253	Modeling and validation of carbon dioxide absorption in aqueous solution of piperazine + methyldiethanolamine by PC-SAFT and E-NRTL models in a packed bed pilot plant: Study of kinetics and thermodynamics. 2020 , 141, 95-109		4
252	Thermodynamic Modeling of Solvent-Impact on Phase Separation in Amorphous Solid Dispersions during Drying. 2020 , 17, 2721-2733		12
251	Xylitol solubility in DMF + ethylene glycol or 1,2-propylene glycol: Measurement and modeling with PC-SAFT and CPA equations of state and UNIFAC activity coefficient model. 2020 , 519, 112651		2
250	Effect of different polymer molar mass on the phase behavior of carbon dioxide dichloromethane Etaprolactone poly (Etaprolactone) system. 2020 , 521, 112687		1
249	Continuum scale modelling of salt precipitation in the context of CO2 storage in saline aquifers with MRST compositional. 2020 , 99, 103075		5
248	A perturbed-chain equation of state based on Wertheim TPT for the fully flexible LJ chains in the fluid and solid phases. 2020 , 152, 134502		2
247	Two-step sub/supercritical water and ethanol processes for non- catalytic biodiesel production. 2020 , 150, 107881		4

246	Hydrate formation in polymer-based pharmaceutical formulations. 2020, 521, 112677		2
245	Experimental PII Data and Modeling for Butan-2-ol + n-Octane or n-Decane in the Ranges of 313.15B53.15 K and 0.1D0 MPa. <i>Journal of Chemical & Data, Engineering Data, 2020, 65, 3848-3865</i>		O
244	Phase behavior of carbon dioxide declaration declarat		1
243	A new multiphase and dynamic asphaltene deposition tool (MAD-ADEPT) to predict the deposition of asphaltene particles on tubing wall. 2020 , 195, 107553		4
242	Enrichment at vapourliquid interfaces of mixtures: establishing a link between nanoscopic and macroscopic properties. 2020 , 39, 319-349		26
241	Equations of state in three centuries. Are we closer to arriving to a single model for all applications?. 2020 , 7, 100060		5
240	Vapor Liquid Equilibria of the Ionic Liquid 1-Hexyl-3-methylimidazolium Triflate (C6mimTfO) with n-Alkyl Alcohols. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 5142-5157		2
239	A general framework for modelling association. 2020 , 513, 112544		О
238	Modeling Highly Cross-Linked Epoxy Resins in Solvents of Different Polarities with PC-SAFT. <i>Industrial & Different Polarities with PC-SAFT.</i> 3-9		7
237	A fast inverse Hankel Transform of first Order for computing vector-valued weight Functions appearing in Fundamental Measure Theory in cylindrical Coordinates. 2020 , 511, 112500		2
236	A new study of associating inhomogeneous fluids with classical density functional theory. 2020 , 118, e1725668		5
235	Phase behavior of pharmaceutically relevant polymer/solvent mixtures. 2020 , 577, 119065		14
234	Estimation of PC-SAFT binary interaction coefficient by artificial neural network for multicomponent phase equilibrium calculations. 2020 , 510, 112486		6
233	Solubility and Pseudo Polymorphic Behavior of Nicotinic Acid in Alcoholic Solutions: Experimental Data and Phase Equilibrium Modeling. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 1319-132	5	2
232	Measurements and modeling of the VLE properties of n-hexadecane in supercritical binary propane+n-butane solvent. 2020 , 510, 112502		4
231	Curvature Corrections Remove the Inconsistencies of Binary Classical Nucleation Theory. 2020 , 124, 04570	1	12
230	Density and Viscosity for Binary Mixtures of the Ionic Liquid 1-Butyl-3-methylimidazolium Tetrafluoroborate with 2-Propanol, N,N-Dimethylacetamide and N,N-Dimethylformamide at 293.15B23.15 K: Experimental and PC-SAFT Modeling. 2020 , 49, 405-421		2
229	The role of molecular interactions on Michaelis constants of ∃-chymotrypsin catalyzed peptide hydrolyses. 2020 , 148, 106142		4

228	Measurement and modeling of poly(vinyl stearate) in supercritical fluids. 2020, 37, 346-352		3
227	Revisiting the treatment of cross-association interactions in oxygenate mixtures with the polar PC-SAFT equation of state. 2021 , 529, 112867		2
226	Modeling fluid phase equilibria of carbon dioxide-methanol binary system. 2021 , 529, 112866		1
225	Modeling liquid absorption of highly cross-linked epoxy resins in aqueous electrolyte solutions. 2021 , 529, 112881		1
224	High-pressure vapor + liquid equilibria for the binary system CO2 + (E)-2-hexenal. 2021 , 168, 105027		1
223	P-ET data and modelling for (2-methylpropan-1-oll-In-octane or n-decane) between 313.15IKB53.15IK and 0.1I20IMPa. 2021 , 152, 106279		O
222	Solvent influence on the phase behavior and glass transition of Amorphous Solid Dispersions. 2021 , 158, 132-142		16
221	Combining crystalline and polymeric excipients in API solid dispersions - Opportunity or risk?. 2021 , 158, 323-335		4
220	Purification of chimeric amine dehydrogenase using a tailor-made aqueous two-phase system - A case study. <i>Journal of Molecular Liquids</i> , 2021 , 323, 114991	6	1
219	Solvent effect on the kinetics of the hydrogenation of n-butyl levulinate to Evalerolactone. <i>Chemical Engineering Science</i> , 2021 , 231, 116315	4.4	7
218	Vapor Pressures and Thermophysical Properties of 1-Heptanol, 1-Octanol, 1-Nonanol, and 1-Decanol: Data Reconciliation and PC-SAFT Modeling. <i>Journal of Chemical & Data</i> , 2021, 66, 805-821	2.8	4
217	Solubility of Carbon Dioxide in Carboxylic Acid-Based Deep Eutectic Solvents. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 702-711	2.8	2
216	Minimum miscibility pressure determination in confined nanopores considering pore size distribution of tight/shale formations. 2021 , 286, 119450		2
215	Thermophysical Properties of Heavy Petroleum Fluids. 2021,		1
214	Application of PC-SAFT EOS for Pharmaceuticals: Solubility, Co-Crystal, and Thermodynamic Modeling. 2021 , 110, 2442-2451		4
213	Measurement and PC-SAFT Modeling of the Solubility of Gallic Acid in Aqueous Mixtures of Deep Eutectic Solvents. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 958-967	2.8	8
212	Combination of monovalent and divalent sites on an associating species: Application to water. <i>AICHE Journal</i> , 2021 , 67, e17146	3.6	1
211	Review of Density Measurements and Predictions of CO2Alkane Solutions for Enhancing Oil Recovery. <i>Energy & Discourt Section</i> 2011, 35, 2914-2935	4.1	4

21 0	High-Pressure Phase Equilibria in an Ethanol/Water Binary System: Experimental Data and Modeling. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 928-946	2.8	
209	A modified cell-to-cell simulation model to determine the minimum miscibility pressure in tight/shale formations. 2021 , 76, 48		2
208	PC-SAFT Modeling of Phase Equilibria Relevant for Lipid-Based Drug Delivery Systems. <i>Journal of Chemical & Delivery Systems</i> , 2021, 66, 1280-1289	2.8	2
207	Density, Speed of Sound, Isentropic Compressibility, and Refractive Index of Ternary Mixtures of Oxygenated Additives and Hydrocarbons (Dibutyl Ether + 1-Butanol + Toluene or Cyclohexane) in Fuels and Biofuels: Experimental Data and PC-SAFT Equation-of-State Modeling. <i>Journal of</i>	2.8	4
206	Thermodynamic and transport properties of binary mixtures containing N-Ethylethanamine and (C5 IC9) 1-Alkanol: PC-SAFT model. 1-8		
205	Experimental Data of Thermophysical Properties of Mixtures of Oxygenated Additives + Hydrocarbon in Fuels and Biofuels: Application of Perturbed Chain-Statistical Associating Fluid and Peng R obinson Equations of State. <i>Journal of Chemical & Data</i> , 2021, 66, 1475-1500	2.8	3
204	Predicting the API partitioning between lipid-based drug delivery systems and water. 2021 , 595, 12026	6	0
203	A Residual Entropy Scaling Approach for Viscosity Based on the GERG-2008 Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 2652-2662	3.9	3
202	Phase Equilibrium and Density of CO + Acetic Acid Systems from 308.15 to 338.15 K and 15 to 45 MPa. 2021 , 6, 6663-6673		
201	Density, Viscosity, and Derivative Properties of Diethylene Glycol Monoethyl Ether Under High Pressure and Temperature. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 1457-1465	2.8	4
200	A novel interfacial thermodynamic model for predicting solubility of nanoparticles coated by stabilizers. 2021 , 31, 103-112		2
199	Stability of Pharmaceutical Co-Crystals at Humid Conditions Can Be Predicted. 2021 , 13,		5
198	Comparative Study of DSC-Based Protocols for API-Polymer Solubility Determination. 2021 , 18, 1742-1	757	4
197	Modeling Interfacial Properties with Spot-DGT-ePC-SAFT for Binary Mixtures Including Ionic Liquid-Based Systems. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 4484-4497	3.9	1
196	A predictive PC-SAFT EOS based on COSMO for pharmaceutical compounds. 2021 , 11, 6405		5
195	Hydrogen solubility in bio-based furfural and furfuryl alcohol at elevated temperatures and pressures relevant for hydrodeoxygenation. 2021 , 290, 120021		7
194	Application of Quantum Chemistry Insights to the Prediction of Phase Equilibria in Associating Systems. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 5992-6005	3.9	2
193	ePC-SAFT advanced - Part I: Physical meaning of including a concentration-dependent dielectric constant in the born term and in the Debye-Hākel theory. 2021 , 535, 112967		11

192	Predicting Deliquescence Relative Humidities of Crystals and Crystal Mixtures. 2021, 26,		2
191	Prediction of salting-out in liquid-liquid two-phase systems with ePC-SAFT: Effect of the Born term and of a concentration-dependent dielectric constant. 2021 , 647, 1305-1314		5
190	Vapor Pressures and Thermophysical Properties of Dimethoxymethane, 1,2-Dimethoxyethane, 2-Methoxyethanol, and 2-Ethoxyethanol: Data Reconciliation and Perturbed-Chain Statistical Associating Fluid Theory Modeling. <i>Journal of Chemical & Chemi</i>	2.8	2
189	Hydrophobic eutectic solvents: Thermophysical study and application in removal of pharmaceutical products from water. 2021 , 411, 128472		9
188	Novel Computational Approach by Combining Machine Learning with Molecular Thermodynamics for Predicting Drug Solubility in Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 92	25 3 -920	58 ¹
187	Assessment of the Perturbed Chain-Statistical Associating Fluid Theory Equation of State against a Benchmark Database of High-Quality Binary-System Data. <i>Industrial & Database of High-Quality Binary-System Data</i> . <i>Industrial & Database </i>	3.9	5
186	A modified perturbed chain-statistical associating fluid theory equation of state for water which includes an association dependent hard sphere diameter. <i>AICHE Journal</i> , 2021 , 67, e17342	3.6	2
185	Solubility of H2S under Haloalkaliphilic Conditions: Experimental Measurement and Modeling with the Electrolyte NRTL Equation. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 9304-9312	3.9	O
184	Thermodynamic Properties of Biogenic Amines and Their Solutions. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 2822-2831	2.8	3
183	Co-Crystal Screening by Vapor Sorption of Organic Solvents. 2021 , 21, 4445-4455		1
183	Co-Crystal Screening by Vapor Sorption of Organic Solvents. 2021, 21, 4445-4455 ePC-SAFT advanced [Part II: Application to Salt Solubility in Ionic and Organic Solvents and the Impact of Ion Pairing. 2021, 537, 112989		8
	ePC-SAFT advanced (Part II: Application to Salt Solubility in Ionic and Organic Solvents and the	3.9	
182	ePC-SAFT advanced [Part II: Application to Salt Solubility in Ionic and Organic Solvents and the Impact of Ion Pairing. 2021 , 537, 112989 Accelerate the ePC-SAFT-DFT Calculation with the Chebyshev Pseudospectral Collocation Method.	3.9	8
182	ePC-SAFT advanced [Part II: Application to Salt Solubility in Ionic and Organic Solvents and the Impact of Ion Pairing. 2021, 537, 112989 Accelerate the ePC-SAFT-DFT Calculation with the Chebyshev Pseudospectral Collocation Method. Industrial & Engineering Chemistry Research, 2021, 60, 9269-9285 Two-Binary-Interaction-Parameter Model for Molecular Solute + Ionic Liquid Solution. Industrial		8
182 181 180	ePC-SAFT advanced [Part II: Application to Salt Solubility in Ionic and Organic Solvents and the Impact of Ion Pairing. 2021, 537, 112989 Accelerate the ePC-SAFT-DFT Calculation with the Chebyshev Pseudospectral Collocation Method. Industrial & Samp; Engineering Chemistry Research, 2021, 60, 9269-9285 Two-Binary-Interaction-Parameter Model for Molecular Solute + Ionic Liquid Solution. Industrial & Samp; Engineering Chemistry Research, 2021, 60, 11490-11501 Effect of Power Plant Capacity on the CAPEX, OPEX, and LCOC of the CO2 Capture Process in		8 2 O
182 181 180	ePC-SAFT advanced [Part II: Application to Salt Solubility in Ionic and Organic Solvents and the Impact of Ion Pairing. 2021, 537, 112989 Accelerate the ePC-SAFT-DFT Calculation with the Chebyshev Pseudospectral Collocation Method. Industrial & Samp; Engineering Chemistry Research, 2021, 60, 9269-9285 Two-Binary-Interaction-Parameter Model for Molecular Solute + Ionic Liquid Solution. Industrial & Samp; Engineering Chemistry Research, 2021, 60, 11490-11501 Effect of Power Plant Capacity on the CAPEX, OPEX, and LCOC of the CO2 Capture Process in Pre-Combustion Applications. 2021, 109, 103371 Insights into the orientation and hydrogen bond influence on thermophysical and transport properties in choline-based deep eutectic solvents and methanol. Journal of Molecular Liquids, 2021	3.9	8 2 0
182 181 180 179	ePC-SAFT advanced [Part II: Application to Salt Solubility in Ionic and Organic Solvents and the Impact of Ion Pairing. 2021, 537, 112989 Accelerate the ePC-SAFT-DFT Calculation with the Chebyshev Pseudospectral Collocation Method. Industrial & Samp; Engineering Chemistry Research, 2021, 60, 9269-9285 Two-Binary-Interaction-Parameter Model for Molecular Solute + Ionic Liquid Solution. Industrial & Samp; Engineering Chemistry Research, 2021, 60, 11490-11501 Effect of Power Plant Capacity on the CAPEX, OPEX, and LCOC of the CO2 Capture Process in Pre-Combustion Applications. 2021, 109, 103371 Insights into the orientation and hydrogen bond influence on thermophysical and transport properties in choline-based deep eutectic solvents and methanol. Journal of Molecular Liquids, 2021, 117019 Hydrogen bond donor and alcohol chain length effect on the physicochemical properties of choline	3.9	8 2 0 7 2

174	Production of polylactic acid aerogels via phase separation and supercritical CO2 drying: thermodynamic analysis of the gelation and drying process. 1		1
173	Densities, viscosities and excess properties for n-nonane with alcohols (C3-C6) from 303.15 k to 333.15 k at atmospheric pressure. <i>Journal of Molecular Liquids</i> , 2021 , 338, 116668	6	O
172	Experimental data and modeling of liquid density, speed of sound, refractive index and derivative properties of ternary mixtures dibutyl ether + 1-butanol + heptane or + methylcyclohexane: Application of PC-SAFT equation of state. 2021 , 161, 106549		3
171	A novel modification of ionic liquid mixture density based on semi-empirical equations using laplacian whale optimization algorithm. 2021 , 14, 103368		1
170	Sequestration of light hydrocarbons in Ionic Liquids at high-pressures: Consistency and thermodynamic modeling. 2021 , 546, 113119		О
169	Phase equilibria of laline/laleucine solid solutions. <i>Journal of Molecular Liquids</i> , 2021 , 340, 117315	6	1
168	Influence of thermal diffusion on the solvent absorption kinetics of highly cross-linked epoxy resins. <i>Journal of Molecular Liquids</i> , 2021 , 339, 116809	6	
167	Experimental and modelled thermophysical behaviour of methyl levulinate (methyl 4-oxopentanoate) and n-alkanol systems. <i>Journal of Molecular Liquids</i> , 2021 , 339, 116739	6	O
166	Hydrodynamic density functional theory for mixtures from a variational principle and its application to droplet coalescence. 2021 , 155, 134101		1
165	Hydrogen solubility equilibria in bio-based Guaiacol or Levulinic acid/water mixture as lignin or cellulose depolymerization model solutions. 2021 , 546, 113115		4
164	Solvent mixtures in pharmaceutical development: Maximizing the API solubility and avoiding phase separation. 2021 , 548, 113200		О
163	Modeling the Vapor-Liquid equilibria of binary and ternary systems comprising associating and non-Associating compounds by using Perturbed-Chain Statistical association fluid Theory. Part I. 2021 , 162, 106563		O
162	Estimation of pure component parameters of PC-SAFT EoS by an artificial neural network based on a group contribution method. 2021 , 548, 113179		O
161	Prediction of dynamic viscosities of carbon dioxide lbrganic solvent mixtures with combined equation of state and Eyring theory. 2021 , 177, 105345		O
160	An effective procedure for wax formation modeling using multi-solid approach and PC-SAFT EOS for petroleum fluids with PNA characterization. 2021 , 207, 109103		2
159	Solubility analysis of pharmaceuticals guaifenesin, ketoprofen, and artemisinin in different solvents. <i>Journal of Molecular Liquids</i> , 2021 , 343, 117503	6	4
158	Predicting process design spaces for spray drying amorphous solid dispersions. 2021 , 3, 100072		2
157	Phase behavior of ASDs based on hydroxypropyl cellulose. 2021 , 3, 100070		6

156	Thermodynamic modeling of trans/supercritical fuel sprays in internal combustion engines based on a generalized cubic equation of state. 2022 , 307, 121894		O
155	Measurement of the density of carbon dioxide/toluene homogeneous mixtures and correlation with equations of state. 2022 , 164, 106618		Ο
154	Thermophysical properties of binary liquid mixtures of oxygenated compounds: 2-Methoxyethanol⊕ alcohols at T 298.15 and 313.15 K. 2022 , 164, 106593		О
153	Methodology Based on the Theory of Information to Describe the Representation Ability of the DMC + Alkane Behavior. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 1036-1054	3.9	2
152	Thermodynamic Modelling of Hydrogel Systems. 2013 , 175-187		4
151	Thermodynamic Modeling of Complex Systems. 2009 , 75-108		15
150	Co-Oriented Fluid Functional Equation for Electrostatic interactions (COFFEE). <i>Chemical Engineering Science</i> , 2017 , 174, 40-55	4.4	11
149	PC-SAFT/UNIQUAC model assesses formation condition of methane hydrate in the presence of imidazolium-based ionic liquid systems. 2020 , 266, 116757		9
148	Predicting the solubilities of metal acetylacetonates in supercritical CO2: Thermodynamic approach using PC-SAFT. 2020 , 164, 104909		5
147	How to Detect Possible Pitfalls in ePC-SAFT Modeling. 2. Extension to Binary Mixtures of 96 Ionic Liquids with CO2, H2S, CO, O2, CH4, N2, and H2. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 21579-21591	3.9	3
146	SAFT-Based MaxwellBtefan Approach to Model the Diffusion through Epoxy Resins. <i>Journal of Chemical & Diffusion through Epoxy Resins</i> . <i>Journal of Chemical & Diffusion through Epoxy Resins</i> . <i>Journal of Chemical & Diffusion through Epoxy Resins</i> . <i>Journal of Chemical & Diffusion through Epoxy Resins</i> .	2.8	3
145	PII Data and Modeling for Butan-1-ol + n-Octane or n-Decane between 313.15B53.15 K and 0.1D0 MPa. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 1636-1654	2.8	3
144	Chapter 8:SAFT Associating Fluids and Fluid Mixtures. 2010 , 215-279		47
143	13 The Role of Molecular Thermodynamics in Developing Industrial Processes and Novel Products That Meet the Needs for a Sustainable Future. 2017 , 633-660		2
142	Modeling of the thermodynamic properties of the methylamine/water refrigerant mixture. 2018, 3,		2
141	Solubility of Polyethylene in n-Hexane and Cyclohexane: Experimental Determination and Comparison with Solid[liquid Equilibria-Based Predictions. <i>Industrial & Determination Chemistry Research</i> , 2021 , 60, 14968-14976	3.9	1
140	Extension of a Group Contribution Method to Predict Viscosity Based on Momentum Transport Theory Using a Modified Peng R obinson EoS. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 14903-14926	3.9	О
139	Phase Equilibria for the Hydroaminomethylation of 1-Decene. <i>Journal of Chemical & December Samp;</i> Engineering Data,	2.8	2

138	The excess volumes of protic ionic liquids and its significance to their thermodynamic modelling. 2022 , 552, 113277	1
137	Prediction of CO2 solubility in electrolyte solutions using the e-PHSC equation of state. 2021 , 180, 105454	O
136	Perturbation Theories for Molecular Fluids. 2013,	
135	Development of a Predictive Molecular Model for Abu Dhabi Crude Oils Phase Behavior. 2018,	
134	Stoffmodelle der Technischen Thermodynamik. 2019 , 1-29	
133	Experimental Density and Viscosity of Aniline and 1-Alkanol Binary Mixtures. <i>Journal of Chemical & Engineering Data</i> ,	
132	Parameterization of a RTPT Association Activity Coefficient Model using Spectroscopic Data. 2021 , 113299	2
131	Modeling the fluid phase behavior of amines, aromatic amines and their mixtures using the modified group-contribution PC-SAFT. 2022 , 551, 113274	1
130	An internally consistent procedure to characterize single carbon number fractions for phase equilibrium of petroleum mixtures: Application to Brazilian pre-salt reservoir fluids. 2021 , 109723	O
129	Phase Equilibrium. 2021 , 177-271	
129	Phase Equilibrium. 2021, 177-271 Interfacial properties of the alkane+water system in the presence of carbon dioxide and hydrophobic silica. 2022, 310, 122332	6
	Interfacial properties of the alkane+water system in the presence of carbon dioxide and	6
128	Interfacial properties of the alkane+water system in the presence of carbon dioxide and hydrophobic silica. 2022, 310, 122332 High-pressure phase behavior of the quaternary system (carbon dioxide lack did in the presence of carbon dioxide lack did in the presence of carbon dioxide lack did in the presence of carbon dioxide and lack did in the presence of carbon dioxide and lack did in the presence of carbon dioxide and hydrophobic silica. 2022, 310, 122332	
128	Interfacial properties of the alkane+water system in the presence of carbon dioxide and hydrophobic silica. 2022, 310, 122332 High-pressure phase behavior of the quaternary system (carbon dioxidel-dichloromethanel-maprolactonel-poly(Etaprolactone): Experimental data and PC-SAFT modeling. 2022, 554, 113306 Activity Coefficients from an Equation of State: Novel Approach for Fast Phase Equilibrium	0
128 127 126	Interfacial properties of the alkane+water system in the presence of carbon dioxide and hydrophobic silica. 2022, 310, 122332 High-pressure phase behavior of the quaternary system (carbon dioxidel-dichloromethanel-daprolactonel-poly(Caprolactone): Experimental data and PC-SAFT modeling. 2022, 554, 113306 Activity Coefficients from an Equation of State: Novel Approach for Fast Phase Equilibrium Calculations. Industrial & Demonstry Research,	2
128 127 126	Interfacial properties of the alkane+water system in the presence of carbon dioxide and hydrophobic silica. 2022, 310, 122332 High-pressure phase behavior of the quaternary system (carbon dioxidel-Idichloromethanel-Itaprolactonel-Ipoly(Etaprolactone): Experimental data and PC-SAFT modeling. 2022, 554, 113306 Activity Coefficients from an Equation of State: Novel Approach for Fast Phase Equilibrium Calculations. Industrial & Dynamic Chemistry Research, 3-9 A van der Waals-EoS-Based Model for the Dynamic Viscosity of Ionic Liquids. 2021, 554, 113343 Isobaric Vaporlliquid Equilibria for the Formic AcidN-methyl-2-pyrrolidone Binary System at 50, 20, and 10 kPa and Modeling Using the NRTL-HOC and PC-SAFT Models. Journal of Chemical & Dynamic Calculations.	2
128 127 126 125	Interfacial properties of the alkane+water system in the presence of carbon dioxide and hydrophobic silica. 2022, 310, 122332 High-pressure phase behavior of the quaternary system (carbon dioxidel-Hichloromethanel-Haprolactonel-Fooly(Haprolactone): Experimental data and PC-SAFT modeling. 2022, 554, 113306 Activity Coefficients from an Equation of State: Novel Approach for Fast Phase Equilibrium Calculations. Industrial & Dynamic Chemistry Research, A van der Waals-EoS-Based Model for the Dynamic Viscosity of Ionic Liquids. 2021, 554, 113343 Isobaric Vaporlliquid Equilibria for the Formic Acid N-methyl-2-pyrrolidone Binary System at 50, 20, and 10 kPa and Modeling Using the NRTL-HOC and PC-SAFT Models. Journal of Chemical & Dynamic Chemical	2

120	Interfacial properties of the aromatic hydrocarbon water system in the presence of hydrophilic silica. <i>Journal of Molecular Liquids</i> , 2022 , 346, 118272	6	3
119	Linear relationships for modeling CO 2 absorption in aqueous alkanolamine solutions in a thermodynamically consistent way. <i>AICHE Journal</i> ,	3.6	
118	Predicting Solvent Effects on Homogeneity and Kinetics of the Hydroaminomethylation: A Thermodynamic Approach Using PC-SAFT. <i>Industrial & Engineering Chemistry Research</i> , 2022 , 61, 2323-2332	3.9	0
117	Solvent Selection for the Extraction of 2-Phenylethanol from Aqueous Phases: Density and Viscosity Studies. <i>Journal of Chemical & Engineering Data</i> ,	2.8	O
116	Interfacial Properties of Deep Eutectic Solvents by Density Gradient Theory. <i>Industrial & Engineering Chemistry Research</i> ,	3.9	1
115	Crossover description of transport properties for some hydrocarbons in the supercritical region. 2022 , 792, 139394		
114	Measurement and modeling of the solubility of ⊞-lactose in water-ethanol electrolyte solutions at 298.15 IK. 2022 , 556, 113378		1
113	Assessment of thermodynamic models via JouleII homson inversion. 2022, 556, 113401		1
112	Evaluation of ePC-SAFT for pH Calculation in Aqueous Itaconic Acid Solutions at High Ionic Strengths. 1		
111	Modelling Subsurface Hydrogen Storage with Transport Properties from Entropy Scaling using the PC-SAFT Equation of State.		1
110	Interfacial Properties of H2O+CO2+Oil Three-Phase Systems: A Density Gradient Theory Study. 2022 , 13, 625		1
109	Extending the Structural (s)-SAFT-IMie Equation of State to Primary Alcohols. <i>Industrial &</i> Engineering Chemistry Research,	3.9	О
108	Water Sorption in Glassy Polyvinylpyrrolidone-Based Polymers 2022 , 12,		2
107	Prediction and correlation of physical properties including transport and interfacial properties with the PC-SAFT equation of state. 2022 , 1-31		
106	Unraveling the influence of dissolved gases on permeate flux in organic solvent nanofiltration appears experimental analysis. 2022 , 121265		0
105	Clapeyron.jl: An Extensible, Open-Source Fluid Thermodynamics Toolkit. <i>Industrial &</i> Engineering Chemistry Research,	3.9	4
104	Steady-State and Dynamic Modeling of the Solution Polyethylene Process Based on Rigorous PC-SAFT Equation of State. <i>Industrial & Engineering Chemistry Research</i> ,	3.9	0
103	High Pressure Vapor Liquid Equilibria of n-Heptane with Ethanol, 1-Propanol, 2-Propanol, and 1-Butanol at 1.5 MPa: Experimental Data of Binary Systems and Perturbed Chain Btatistical Associating Fluid Theory Model Predictions. <i>Journal of Chemical & Che</i>	2.8 1 0-115 6	

102	A study on mixing properties of binary mixtures of 1-hexene with alkoxyethanols at different temperatures. 2022 , 106820		О
101	A rigorous approach for characterising the limiting optimal efficiency of working fluids in organic Rankine cycles. 2022 , 124191		
100	Modeling the solubility of non-steroidal anti-inflammatory drugs (ibuprofen and ketoprofen) in supercritical CO2 using PC-SAFT. 2022 , 186, 105626		О
99	Theoretical modeling and prediction of biorelevant solubility of poorly soluble pharmaceuticals. 2022 , 444, 136678		O
98	Vapor-Liquid equilibria of the systems 1-octanol/nitrogen and 1-octanol/oxygen at pressures from 3 to 9IMPa and temperatures up to 613IK IMeasured in a microcapillary with Raman spectroscopy. 2022 , 323, 124352		
97	Predicting the Thermodynamics of Ionic Liquids: What to Expect from PC-SAFT and COSMO-RS?. 2022 ,		O
96	PCBAFT modeling of the high pressure VLE data for 2,2,4\textbf{II} rimethylpentane with Ethanol, 1\textbf{P} ropanol, 2\textbf{P} ropanol and 1\textbf{B} utanol. Experimental equipment and binary systems at 1.5 MPa. 2022, 106816		
95	Simplified Choice of Suitable Excipients within Biologics Formulation Design using Protein-Protein Interaction- and Water Activity-Maps. 2022 ,		O
94	Parametrization of PC-SAFT EoS for Solvents Reviewed for Use in Pharmaceutical Process Design: VLE, LLE, VLLE, and SLE Study. <i>Industrial & Engineering Chemistry Research</i> ,	3.9	О
93	Modeling VLE and LLE of Deep Eutectic Solvents (DES) and Ionic Liquids (IL) Using PC-SAFT Equation of State. Part II. <i>AICHE Journal</i> ,	3.6	
92	Solubility of Electrolytes in Organic Solvents: Solvent-Specific Effects and Ion-Specific Effects. Journal of Chemical & Data,	2.8	O
91	Surface anomalies in ethanol plus n-octane mixture: An effect of molecular orientations and hydrogen bonds. <i>Journal of Molecular Liquids</i> , 2022 , 361, 119630	6	
90	Mass transfer modeling and sensitivity study of low-temperature Fischer-Tropsch synthesis. <i>Chemical Engineering Science</i> , 2022 , 259, 117774	4.4	0
89	Density Measurements of Homogeneous Phase Fluid Mixtures Comprising Co2/Methanol and Co2/Ethanol Binary Systems and Correlation with Equations of State. SSRN Electronic Journal,	1	
88	Heavy Petroleum Supercritical Fluid Deasphalting Process Simulation Based On the Saturate, Aromatic, Resin, and Asphaltene Composition. <i>Energy & Energy & E</i>	4.1	1
87	Thermodynamic properties of water from SAFT and CPA equations of state: A comprehensive assessment. <i>Journal of Molecular Liquids</i> , 2022 , 362, 119769	6	O
86	A new thermodynamic method to estimate surface tension of liquids. <i>Physica B: Condensed Matter</i> , 2022 , 643, 414178	2.8	0
85	A Thermodynamic Approach for Simultaneous Solvent, Coformer, and Process Optimization of Continuous Cocrystallization Processes. 2022 , 2179-2184		

84	Applications of an Association Activity Coefficient Model, NRTL-PA, to Alcohol-Containing Mixtures.	3
83	Application of Renormalization Corrections to SAFT-VR Mie.	1
82	Application of the PC-SAFT Equation of State to the Prediction of Vapor Solubility in Semi-crystalline Polyethylenes. 2200017	
81	Estimating the solubility of salsalate in supercritical CO2 via PC-SAFT modeling using its experimental solubility data in organic solvents. 2022 , 105725	O
80	Simultaneous Solvent Selection and Process Design for Continuous Reaction Extraction Trystallization Systems. 2022 , 61, 11504-11517	О
79	Effects of mixing and molecular packing on the isobaric expansivity of mixtures of n-hexane and 1-hexanol as modelled by FT-EoS, PC-SAFT and SAFT-IMie. 2022 , 120165	
78	Thermophysical properties of hydrogen mixtures relevant for the development of the hydrogen economy: Review of available experimental data and thermodynamic models. 2022 ,	0
77	Phase Equilibrium of Cross-Associating Mixtures Using Association Theory-Based Equation of State.	3
76	Crude oil wax: A review on formation, experimentation, prediction, and remediation techniques. 2022 ,	O
75	Water adsorption on planar interfaces: classical density functional study. 2022 , 113567	
74	Investigation of carbon dioxide solubility in various families of deep eutectic solvents by the PC-SAFT EoS. 10,	
73	A thermodynamic approach for predicting thermodynamic phase behaviors of pharmaceuticals in biorelevant media. 2022 , 261, 117973	
72	Efficient Implementation of Wertheim Theory: 2. Master Equations for Asymmetric Solvation.	1
71	Compatibility of selected active pharmaceutical ingredients with poly(D, L-lactide-co-glycolide): Computational and experimental study. 2022 , 179, 232-245	2
70	Influence of solvent and salt on kinetics and equilibrium of esterification reactions. 2022, 263, 118046	1
69	Infrared quantification of ethanol and 1-butanol hydrogen bonded hydroxyl distributions in cyclohexane. 2023 , 285, 121837	1
68	Crossover PC-SAFT equations of state based on White's method for the thermodynamic properties of CO2, n-alkanes and n-alkanols. 2023 , 564, 113610	О

66	The monotonicity behavior of density profiles at vapor-liquid interfaces of mixtures. 2023, 564, 113596	3
65	Experimental data and thermodynamic modeling of the CO214 (Acetone (4) Efavirenz system at high pressures. 2023 , 176, 106924	O
64	Parametrization of the NRTL Model with a Multiobjective Approach: Implications in the Process Simulation. 2022 , 2, 267-288	0
63	Multi-objective optimization of equation of state molecular parameters: SAFT-VR Mie models for water. 2022 , 108015	O
62	Purely Predicting the Pharmaceutical Solubility: What to Expect from PC-SAFT and COSMO-RS?.	1
61	Explaining the Release Mechanism of Ritonavir/PVPVA Amorphous Solid Dispersions. 2022, 14, 1904	O
60	Assessing the Influence of Betaine-Based Natural Deep Eutectic Systems on Horseradish Peroxidase. 2022 , 10, 12873-12881	0
59	Solubility of CO2 in Ionic Liquids with Additional Water and Methanol: Modeling with PC-SAFT Equation of State. 2022 , 61, 14364-14373	1
58	Study of Density and Viscosity of Formic Acid + 1-Alkanols Mixtures: Application of PC-SAFT Model. 2022 , 43,	0
57	Electrolyte Thermodynamic Models in Aspen Process Simulators and Their Applications.	1
56	Pore-network modeling of flow in shale nanopores: Network structure, flow principles, and computational algorithms. 2022 , 104203	1
55	Thermodynamic modeling of gas solubility in ionic liquids using equations of state. 2022 , 28-28	O
54	Osmolyte Effect on Enzymatic Stability and Reaction Equilibrium of Formate Dehydrogenase.	1
53	Wertheim Association Theory for Phase Equilibrium Modeling in Chemical Engineering Practice. 2022 , 61, 15678-15713	2
52	Analysis of Vaporlliquid Interfacial Transport Resistivities with DGT-PC-SAFT Based on the General Approach.	0
51	Strategy for Fast Decision on Material System Suitability for Continuous Crystallization Inside a Slug Flow Crystallizer. 2022 , 13, 1795	2
50	Vapor-liquid equilibrium for the {R-OHI-IR-palmitate} systems at 50.3 and 101.3IkPa. 2023 , 333, 126459	0
49	Calculation of azeotropic properties for binary mixtures with the PC-SAFT equation of state. 2023 , 565, 113631	O

48	Group-Contribution SAFT Equations of State: A Review. 2022 , 113674	1
47	Thermodynamic and Transport Properties of Formic Acid and 2-Alkanol Mixtures: PC-SAFT Model.	O
46	Experimental optimization of the supercritical fluid extraction of triterpenoids from Acacia dealbata Link. leaves. 2022 , 122637	1
45	Density, Viscosity, Refractive Index, and Related Thermophysical Properties of Dibutyl Ether +2-Butanol + Cyclohexane Ternary Systems.	O
44	Thymol+l-menthol eutectic mixtures: Thermophysical properties and possible applications as decontaminants. 2022 , 120789	1
43	Simultaneous Optimization of Process Design and Solvent in a Flowsheet Simulator.	O
42	Interfacial behaviors of the H2O+CO2+CH4+C10H22 system in three phase equilibrium: A combined molecular dynamics simulation and density gradient theory investigation. 2023 , 370, 121031	0
41	Miscibility of Poly(lactide-co-glycolide) in Supercritical fluids. 2023 , 369, 120853	O
40	Beyond FloryHuggins: Activity Coefficients from Perturbation Theory for Polar, Polarizable, and Associating Solvents to Polymers. 2022 , 61, 17644-17664	O
39	Thermodynamic characterization of the (H2 + C3H8) system significant for the hydrogen economy: Experimental (p, \Box T) determination and equation-of-state modelling. 2022 ,	O
38	Prediction of solubility of vitamins in the mixed solvents using equation of state. 2022, 113715	O
37	Predicting CO2 solubility in aqueous and organic electrolyte solutions with ePC-SAFT advanced. 2022 , 113714	1
36	Toward Advanced, Predictive Mixing Rules in SAFT Equations of State. 2022, 61, 18165-18175	O
35	Investigation of the Antisolvent Effect on the Phase Behavior of Amino Acid Solid Solutions.	O
34	Interfacial properties of the hexane + carbon dioxide + water system in the presence of hydrophilic silica. 2022 , 157, 234704	0
33	A Multi-Criteria Study of Optimal Working Fluids for High Temperature Heat Pumps.	O
32	Ion-dipole complex effect on activity coefficient of L-methionine in aqueous NaCl and NaNO3 solutions.	О
31	The Thermodynamic Properties of Non-Associating and Associating Fluids: A Systematic Evaluation of SAFT-Type Equations of State. 2023 , 44,	Ο

30	Thermodynamic Mechanism of Physical Stability of Amorphous Pharmaceutical Formulations.	0
29	A Workflow for Crystallization Process Design with Simultaneous Process Optimization and Solvent Selection based on the Perturbed-Chain Statistical Associating Fluid Theory.	O
28	Miscibility in systems containing (poly(oxymethylene) ethers (OME) [hydrocarbons [hater]. 2023 , 338, 127337	O
27	Dualistic Role of Alcohol in Micelle Formation and Structure from iSAFT Based Density Functional Theory and COSMOplex. 2023 , 62, 1968-1983	O
26	Simultaneous Predictions of Chemical and Phase Equilibria in Systems with an Esterification Reaction Using PC-SAFT. 2023 , 28, 1768	О
25	The Effect of Binary Interaction Parameters and Induced Association on the Performance of the PC-SAFT Equation of State: Validation against a Benchmark Database of High-Quality Binary-System Data.	О
24	Solid Liquid Equilibrium in Co-Amorphous Systems: Experiment and Prediction. 2023, 28, 2492	0
23	Interfacial tension of water near to critical conditions by using the pendant drop method: New experimental data and a correlation based on the parachor method. 2023 , 196, 105899	O
22	Accounting for cross-association in nonself-associating species using SAFT-VR Mie: Application to mixtures with esters. 2023 , 569, 113775	О
21	Modeling and prediction of thermodynamic phase behaviors of oxaprozin and irbesartan in biorelevant media. 2023 , 571, 113806	O
20	Theoretical and experimental study of triethanolamine and 1-alkanol mixtures. 2023, 571, 113810	0
19	Systematic evaluation of parameterization approaches for the ePPC-SAFT model for aqueous alkali halide solutions. 2023 , 570, 113778	О
18	Multicomponent diffusivities in supercritical and liquid ternary systems. 2023, 196, 105881	0
17	Interfacial tension and phase equilibria for binary systems containing (CH4-CO2)+(n-dodecane; n-butanol; water). 2023 , 570, 113783	0
16	Aromatic volatile organic compounds absorption with phenyl-based deep eutectic solvents: A molecular thermodynamics and dynamics study. 2023 , 69,	0
15	Dry glass reference perturbation theory predictions of the pervaporation separation of solvent mixtures using PIM-1 membranes. 2023 , 672, 121420	O
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13	Effect of Copolymer Properties on the Phase Behavior of Ibuprofen B LA/PLGA Mixtures. 2023 , 15, 645	О

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2	High-pressure densities of 2-(Dimethylamino) ethanol and 2-(Diethylamino) ethanol: Measurement and modeling with new modified Tait and PC-SAFT equations of state. 2023 , 113825	0
1	Modeling the temperature-dependent solubility of salts in organic solvents. 2023 , 113828	o