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2282	THE UNIFAC GROUP-CONTRIBUTION METHOD. 1977 , 27-64		96
2281	INTRODUCTION. 1977 , 1-5		10
2280	Thermodynamik fl Ssiger Mischungen von Kohlenwasserstoffen mit verwandten Substanzen. 1977 , 81, 908-921		84
2279	Analysis of a complex plant-steady state and transient behavior. 1977 , 1, 75-100		61
2278	Qualities of models for evaluation, representation and prediction of fluid phase equilibrium data. <i>Fluid Phase Equilibria</i> , 1978 , 2, 101-118	2.5	6
2277	Prediction of the excess enthalpies of mixing of mixtures using the UNIFAC method. 1978 , 33, 177-182		21
2276	Prediction of Separation Factors Using Group Contribution Methods a Review. 1978 , 7, 147-182		7

2275	Nahordnung in Fl\(\Big \) \(\text{Sigkeiten}, VII. Additivit\(\Displies\) \(\text{tseffekte in mehrfach chlorsubstituierten Benzolen.}\) 1978 , 82, 457-462	3
2274	A predictive method for calculating the solubility of solids in supercritical gases application to apolar mixtures. 1979 , 34, 1393-1400	6
2273	Isothermal vaporliquid equilibria for two binary mixtures of heptane with 2-butanone and 4-4-methyl-2-pentanone measured by a dynamic still with a pressure regulation. <i>Fluid Phase Equilibria</i> , 1979 , 3, 123-131	25
2272	Heats of mixing of amine-alcohol systems. An analytical group solution model approach. 1979 , 57, 355-362	10
2271	Bibliography. 1979 , 386-440	
2270	Auswahl von L\[Bungsmitteln f\[Bidie Extraktiv-Rektifikation mittels vorausberechneter Gleichgewichtsdaten. 1979, 83, 1133-1136	18
2269	Absch Ezung des L Eungsmitteleffektes auf die Geschwindigkeit chemischer Reaktionen mit Hilfe der UNIFAC-Methode. 1980 , 122, 251-254	3
2268	Lattice-model expressions for the combinatotial entropy of liquid mixtures: A critical discussion. 1980 , 19, 1-10	29
2267	Anwendung der Mischphasen-Thermodynamik auf die Berechnung von thermischen Stofftrennverfahren. 1980 , 52, 209-218	3
2266	On the temperature dependence of the UNIQUAC/UNIFAC models. 1980 , 35, 2389-2403	71
2265	Thermodynamische Untersuchungen von Polymerl Bungen mit der Fl Bsig-Gas-Chromatographie. 1980 , 31, 377-381	3
2264	Thermodynamically based analysis and synthesis of chemical process systems. 1980 , 5, 955-966	13
2263	Liquid-liquid equilibrium data: Their retrieval, correlation and prediction Part III: Prediction. <i>Fluid Phase Equilibria</i> , 1980 , 4, 151-163	57
2262	A simplified group method analysis. <i>Fluid Phase Equilibria</i> , 1980 , 4, 211-228 2.5	13
2261	On the combinatorial part of the UNIFAC and UNIQUAC models. 1980 , 58, 253-258	170
2260	Engineering Aspects of Gas-Liquid Catalytic Reactions. 1980 , 22, 75-140	23
2259	RECENT PROGRESS IN THE COMPUTATION OF EQUILIBRIUM RATIOS. 1980 , 4, 485-500	6
2258	The thermodynamic properties of fluid mixtures. 1981 , 13-14, 41-64	5

2257	WATER ACTIVITY AND ITS ESTIMATION IN FOOD SYSTEMS: THEORETICAL ASPECTS. 1981, 1-61		173
2256	Anwendung der Unifac-Methode zur Vorausberechnung von Extraktionsparametern. 1981 , 53, 542-540	6	9
2255	Extraction with supercritical gases. 1981 , 36, 1769-1788		192
2254	Phase Equilibria by effective UNIFAC group-contribution method. 1981 , 48, 187-211		10
2253	Thermodynamic properties of binary mixtures containing ketones. VI. Analysis of the properties of 2-propanone + n-alkane mixtures in terms of a quasi-chemical group contribution model. <i>Fluid Phase Equilibria</i> , 1981 , 5, 159-189	2.5	40
2252	Solution thermodynamics for Eleactive Ecomponents. Fluid Phase Equilibria, 1981, 5, 245-277	2.5	17
2251	Prediction of excess gibbs energy and excess enthalpy on the basis of non-analytical solution-of-groups concept. <i>Fluid Phase Equilibria</i> , 1981 , 6, 61-81	2.5	7
2250	A note on excess Gibbs energy models, equations of state and the local composition concept. <i>Fluid Phase Equilibria</i> , 1981 , 7, 121-138	2.5	93
2249	Measurement, correlation and estimation of binary vaporliquid equilibria for alcoholihlorobenzene systems. <i>Fluid Phase Equilibria</i> , 1981 , 7, 29-40	2.5	4
2248	Local compositions and local surface area fractions: A theoretical discussion. 1981 , 59, 501-505		74
2247	THE EFFECT OF SOLUTES ON BUBBLE SIZE IN AIR-WATER DISPERSIONS. 1982, 17, 85-98		41
2246	UNIFAC and infinite dilution activity coefficients. 1982 , 60, 300-304		13
2245	Inhibition of bubble coalescence by solutes in air/water dispersions. 1982 , 37, 1635-1638		118
2244	On the concentration dependence of the UNIQUAC/UNIFAC models. 1982 , 37, 99-111		34
2243	LiquidIquid equilibria for the system water + acetic acid + methyl isoamyl ketone. <i>Fluid Phase Equilibria</i> , 1982 , 9, 177-185	2.5	7
2242	Correlation for the ratio of limiting activity coefficients for binary liquid mixtures. <i>Fluid Phase Equilibria</i> , 1982 , 8, 149-160	2.5	2
2241	Isothermal measurements of vapor-liquid equilibria for three n-alkane-chloroalkane mixtures. <i>Fluid Phase Equilibria</i> , 1982 , 8, 285-300	2.5	30
2240	Prediction of vapour-liquid equilibria for systems containing longer-chain alcohols and alkanes by various group-contribution methods. <i>Fluid Phase Equilibria</i> , 1982 , 9, 67-77	2.5	4

2239	Remarks on molecular approaches to liquid mixtures. <i>Fluid Phase Equilibria</i> , 1983 , 10, 1-7 2.5	24
2238	Liquid-liquid equilibria of the system water-isobutyric acid-cumene. Fluid Phase Equilibria, 1983, 15, 91-1055	8
2237	Vapor-liquid equilibria of strong electrolytes in systems containing mixed solvent. <i>Fluid Phase Equilibria</i> , 1983 , 13, 311-319	33
2236	Molecular design of solvents for liquid extraction based on UNIFAC. Fluid Phase Equilibria, 1983, 13, 331-24.40) 167
2235	Liquid I quid and vapour I quid equilibrium data and calculations for the system aniline + water in the presence of NaCl, NaI, NH4Cl and NH4I. Fluid Phase Equilibria, 1983, 11, 91-102	9
2234	Calorimetry: Its contributions to molecular thermodynamics of fluids. 1983 , 69, 1-44	17
2233	Utilization of the solution-of-groups concept in gas[]quid chromatography. 1983, 258, 23-33	15
2232	Solubility in binary solvent systems. IV. Prediction of naphthalene solubilities using the UNIFAC group contribution model. 1983 , 13, 197-204	28
2231	Identification of Additives to Render Mixtures of Gasoline and the Ethanol-Water Azeotrope Hiscible. 1983 , 12, 143-176	
2230	Prediction of Gas Solubilities by a Modified UNIFAC-Equation. 1983 , 87, 17-23	25
2230	Prediction of Gas Solubilities by a Modified UNIFAC-Equation. 1983 , 87, 17-23 References. 1984 , 287-294	25
2229		25 1
2229	References. 1984 , 287-294	
2229	References. 1984 , 287-294 Distillation: Research Needs. 1984 , 19, 943-961	1
2229	References. 1984, 287-294 Distillation: Research Needs. 1984, 19, 943-961 A liquid-liquid extractor model based on UNIFAC. 1984, 8, 127-136 Measurement, correlation and prediction of binary vapor-liquid equilibria for	1 4
2229 2228 2227 2226	References. 1984, 287-294 Distillation: Research Needs. 1984, 19, 943-961 A liquid-liquid extractor model based on UNIFAC. 1984, 8, 127-136 Measurement, correlation and prediction of binary vapor-liquid equilibria for alcohol-tetrachloroethene systems. 1984, 62, 142-148	1 4
2229 2228 2227 2226	References. 1984, 287-294 Distillation: Research Needs. 1984, 19, 943-961 A liquid-liquid extractor model based on UNIFAC. 1984, 8, 127-136 Measurement, correlation and prediction of binary vapor-liquid equilibria for alcohol-tetrachloroethene systems. 1984, 62, 142-148 Solubility of biphenyl in binary solvent mixtures. 1984, 18, 47-52	1 4 1 29

2221	VAPOR-LIQUID EQUILIBRIA PREDICTION FOR SYSTEMS CONTAINING UNSATURATED HYDROCARBONS THE UNIFAC MODEL FOR PREDICTING BOILING TEMPERATURE. 1984 , 26, 105-110	1
2220	Correlations for the solubility of normal alkanoic acids ando-toluic acid in binary solvent mixtures. 1985 , 14, 531-547	39
2219	Pure-component vapour pressures of heavy hydrocarbons containing nitrogen or sulphur using the UNIFAC group-contribution method. <i>Fluid Phase Equilibria</i> , 1985 , 24, 177-186	1
2218	The generalized van der waals partition function. I. basic theory. <i>Fluid Phase Equilibria</i> , 1985 , 19, 238-257 _{2.5}	100
2217	From Redlich-Kister to local composition models, group solutions, and electrolytes. <i>Fluid Phase Equilibria</i> , 1985 , 24, 77-85	1
2216	NRTL: An empirical equation or an inspiring model for fluids mixtures properties?. <i>Fluid Phase Equilibria</i> , 1985 , 24, 87-114	13
2215	From UNIFAC to SUPERFAC - and back?. Fluid Phase Equilibria, 1985, 24, 115-150 2.5	37
2214	Adsorption from multi-component liquid mixtures on to heterogeneous solid surfaces: the role of adsorption of water on silica in liquidBolid adsorption chromatography. 1985 , 348, 1-25	10
2213	Utilization of the functional group contribution concept in liquid chromatography on chemically bonded reversed phases. 1985 , 348, 49-65	18
2212	Vapor-liquid equilibria of {xCH3CH(CH3)CHO+(1☒)C7H16}(l) and {xCH3CO2C2H5+(1☒)C7H16}(l). 1985 , 17, 143-150	16
2211	Excess enthalpies between 293 and 323 K for constituent binaries of ternary mixtures exhibiting partial miscibility. 1985 , 17, 719-732	46
221 0	Excess enthalpies of mixing using a modified AGSM approach. 1985 , 84, 247-254	
2209	Screening and identification of extractive fermentation solvents using a database. 1985 , 63, 919-927	59
2208	The prediction of vapor-liquid equilibrium from heat of mixing data for binary nitrile-alcohol mixtures. 1985 , 91, 37-51	5
2207	A semi-empirical method for the prediction of the volumetric behaviour of pure fluids. 1985 , 40, 995-1002	4
2206	Prediction of solubility in nonideal multicomponent systems using the UNIFAC group contribution model. 1985 , 74, 634-7	21
2205	Aromatic Compound Solubility in Solvent/Water Mixtures. 1986, 112, 328-345	60
2204	Recovery of n-Butanol from Dilute Solution by Extraction. 1986 , 21, 1059-1074	6

2203	Local composition models in pharmaceutical chemistry. III. Prediction of drug solubility in binary aqueous mixtures. 1986 , 32, 187-198		2
2202	Evaporative Emissions from Gasolines and Alcohol-Containing Gasolines with Closely Matched Volatilities. 1986 ,		25
2201	Analysis of the Dynamic Behavior of Distillation Trains. 1986 , 19, 105-110		1
2200	Optimization of polymer-solvent interaction in a multisolvent system by the UNIFAC group-contribution method. 1986 , 32, 5007-5019		5
2199	Mathematical model of extractive fermentation: application to the production of ethanol. 1986 , 28, 1206	-12	23
2198	Perfluorodecaline/hydrocarbon systems prediction and correlation of liquid l lquid equilibrium data. <i>Fluid Phase Equilibria</i> , 1986 , 25, 291-302	5	4
2197	Evaluation of the methods of correlation and interpolation of quaternary liquid equilibrium data. Application to the system water ## than old horoform ## louene at 25°C. Fluid Phase 2 Equilibria, 1986, 25, 147-160	5	2
2196	The application of fuzzy set theory to uncertainty in physical property models. <i>Fluid Phase Equilibria</i> , 1986 , 30, 111-118	:.5	1
2195	Group contribution methods for the estimation of activity coefficients. <i>Fluid Phase Equilibria</i> , 1986 , 30, 119-134	5	15
2194	Integral equation group contribution methods. <i>Fluid Phase Equilibria</i> , 1986 , 30, 143-148	:.5	
2193	Prediction of viscosities of liquid mixtures by a group contribution method. <i>Fluid Phase Equilibria</i> , 1986 , 30, 149-156	5	73
2192	Vapourliquid equilibrium of the system benzene + cyclohexane + 1-propanol at 760 mm Hg. <i>Fluid Phase Equilibria</i> , 1986 , 26, 69-81	:.5	2
2191	A strategy for the design and selection of solvents for separation processes <i>Fluid Phase Equilibria</i> , 1986 , 29, 125-132	5	96
2190	Experimental solid-liquid equilibria of binary mixtures of organic compounds. <i>Fluid Phase Equilibria</i> , 1986 , 29, 265-272	5	5
2189	Computer simulation of fluid mixtures. <i>Fluid Phase Equilibria</i> , 1986 , 29, 307-325	5	10
2188	Density dependent local composition models: an interpretive review. <i>Fluid Phase Equilibria</i> , 1986 , 29, 415-430	5	12
2187	Extension of UNIFAC to high pressure VLE using Vidal mixing rules. Fluid Phase Equilibria, 1986, 28, 155-12	7.9	11
2186	Vapor-liquid equilibria for binary mixtures of carbon dioxide with benzene, toluene and p-xylene. Fluid Phase Equilibria, 1986 , 31, 299-311	5	71

2185	Separations from Dilute Solutions: Group-contribution methods. <i>Fluid Phase Equilibria</i> , 1986 , 27, 347-372 _{.5}	3
2184	Prediction of solubility of long-chain hydrocarbons in various solvents using UNIFAC. 1986 , 7, 319-330	7
2183	Importance of thermophysical data in process simulation. 1986 , 7, 987-1002	2
2182	Factors affecting adsorption of organic solutes on cellulose acetate in an aqueous solution system. 1986 , 22, 55-58	42
2181	A modified Inside-outlalgorithm for simulation of multistage multicomponent separation processes using the UNIFAC group-contribution method. 1986 , 64, 759-767	5
2180	Vaporliquid equilibria of acetonitrile-1-propanol mixtures. 1986 , 64, 813-819	8
2179	Prediction of ternary liquid-liquid equilibria using the NRTL and the UNIQUAC models. 1986 , 3, 141-151	4
2178	Chemical Engineering Thermodynamics: Education and Application. 1986 , 11,	
2177	Thermochemical Investigations of Associated Solutions. 3. Effect of the Inert Cosolvent on Solute-Solvent Association Constants Calculated from Solubility Measurements. 1987 , 17, 123-138	43
2176	Dynamic simulation of liquid[]quid operations using simple non-linear models. 1987, 11, 177-185	3
2175	Application of NRTL and uniquac models to liquid-liquid systems with halogen salts (Part I). 1987 , 4, 161-169	0
2174	A diffusion coefficient model for polymer devolatilization. 1987 , 27, 303-312	3
2173	The importance of enthalpic interactions in polymeric systems. 1987 , 27, 1482-1494	41
2172	A one-parameter group-contribution model for liquid mixtures. 1987 , 16, 625-634	2
2171	Unifac interaction parameters for excess enthalpies of mixing. 1987 , 111, 267-274	3
2170	Prediction of thermodynamic properties of polymer solutions using the UNIFAC group-contribution method. 1987 , 28, 2105-2109	5
2169	Phase equilibria in very dilute mixtures of water and chlorinated hydrocarbons. Part IIŪnifac parameters. <i>Fluid Phase Equilibria</i> , 1987 , 35, 207-215	5
2168	Liquid I quid equilibria of the system water + acetic acid + methyl ethyl ketone at several temperatures. Fluid Phase Equilibria, 1987, 32, 151-162	18

2167	A group-contribution, continuous-thermodynamics framework for calculation of vapor-liquid equilibria. 1987 , 65, 651-661	7	
2166	Extractive Fermentation of Acetone and Butanol: Process Design and Economic Evaluation. 1987 , 3, 131-140	81	
2165	Selectivity in a liquid-solid chromatographic system. 1987 , 24, 800-804	2	
2164	Solute retention in the stationary phase of a liquid-solid chromatographic system. 1987 , 23, 915-924	4	
2163	Water solubility: a critique of the solvatochromic approach. 1988, 77, 74-7	21	
2162	Auswahl und Auslegung thermischer Trennprozesse mit Hilfe von Gruppenbeitragsmethoden. 1988 , 60, 759-768	4	
2161	Sensitivity testing with the predictive thermodynamic models NRTL, UNIQUAC, ASOG and UNIFAC in multicomponent separations of methanol-acetone-chloroform. 1988 , 43, 495-501	4	
2160	Narrow-boiling distillates of coal liquefaction products: 1. Functional group distributions. 1988 , 67, 119-126	13	
2159	Group contribution methods for coal-derived liquids: hydrogen solubilities using a UNIFAC approach. 1988 , 67, 1609-1614	11	
2158	Vaporliquid equilibria of 2-propanol + water + N,N-dimethyl formamide. <i>Fluid Phase Equilibria</i> , 1988, 43, 77-89	33	
2157	Solubility of 2,5-dimethylphenol and 3,4-dimethylphenol in binary solvent mixtures containing alcohols. <i>Fluid Phase Equilibria</i> , 1988 , 40, 259-277	12	
2156	Solubility of anthracene in binary solvent mixtures containing tetrahydropyran. <i>Fluid Phase Equilibria</i> , 1988 , 41, 187-194	3	
2155	Mutual binary solubilities: perfluoromethylcyclohexaneflydrocarbons. <i>Fluid Phase Equilibria</i> , 1988 , 41, 205-214	3	
2154	Vaporliquid equilibrium calculations of multicomponent systems based on Taylor series approximation for quasichemical equilibria. <i>Fluid Phase Equilibria</i> , 1988 , 43, 57-71	3	
2153	Group contribution methods for molecular mixtures. I. Interaction site models. <i>Fluid Phase Equilibria</i> , 1988 , 43, 231-261	6	
2152	Binary and ternary vapor[Iquid equilibrium calculations for methyl chloride, dimethyl ether and methanol. 1988 , 24, 57-62	2	
2151	An iso-propanol distillery revamping using a simbad simulator. 1988 , 12, 807-819	1	
2150	Heat of mixing of R22-absorbent mixtures. 1988 , 11, 92-95	9	

2149	Liquid-liquid equilibria of the system water + acetic acid + methyl propyl ketone. 1988 , 66, 136-140		6
2148	Prediction and experimental determination of vapour-liquid equilibria for benzene + Cyclohexane + 1-Butanol mixtures at 101.325 kPa. 1988 , 66, 452-457		1
2147	Solubility of Anthracene in Binary p-xylene + Alkane and Benzene + Alkane Solvent Mixtures. 1989 , 20, 31-38		10
2146	Selectivity in Reversed-Phase Liquid Chromatography. 1989 , 12, 59-75		7
2145	A SEMI-EMPIRICAL MOLECULAR ACTIVITY COEFFICIENT MODEL WITH IRREGULAR PARAMETER DISTRIBUTION. 1989 , 80, 127-134		4
2144	The Solubility of Amino Acids in Mixtures of Water and Aliphatic Alcohols. 1989 , 5, 89-91		29
2143	Correlation between retention and the C18 silica surface coverage in reversed-phase liquid chromatography. 1989 , 27, 378-384		12
2142	A cubic equation of state for predicting vaporllquid equilibria of hydrocarbon mixtures using a group contribution mixing rule. <i>Fluid Phase Equilibria</i> , 1989 , 46, 197-210	2.5	10
2141	Fluid phase equilibrium and volumetric properties from the Chain-of-Rotators group contribution equation of state. <i>Fluid Phase Equilibria</i> , 1989 , 51, 147-159	5	11
2140	Chain-of-rotators group contribution equation of state. 1989 , 44, 2553-2564		41
2139	Prediction of retention in gasIlquid chromatography using the unifac group contribution method. 1989 , 483, 1-19		9
2138	Prediction of vapour-liquid equilibria of mixtures containing keto-enol tautomers and solvent. <i>Fluid Phase Equilibria</i> , 1989 , 49, 151-156	2.5	4
2137	Solubility of n-alkanols (C16,C18,C20) in binary solvent mixtures. Fluid Phase Equilibria, 1989, 46, 223-24&	5	48
2136	Application of the group contribution concept to the Kihara potential for the calculation of second virial coefficients. <i>Fluid Phase Equilibria</i> , 1989 , 47, 47-65	2.5	9
2135	Vapor-liquid equilibria of binary system based on pine resin. <i>Fluid Phase Equilibria</i> , 1989 , 53, 15-22	5	17
2134	An improved mosced equation for the prediction and application of infinite dilution activity coefficients. <i>Fluid Phase Equilibria</i> , 1989 , 52, 151-160	2.5	22
2133	An application of the universal functional group activity coefficient model to electrosorption. 1989 , 262, 263-276		3
2132	Prediction of the solubility of hydrocarbons in water using UNIFAC. 1989 , 24, 49-56		O

2131	Solubility of Anthracene in Binary Carbon Tetrachloride + Alkane Solvent Mixtures. 1989 , 19, 73-79		7	
2130	Fluids in the Gravitational Field Exact Treatment of One Dimensional Systems. 1989 , 93, 870-873		1	
2129	Phase Transition and Equilibrium. 1989 , 22, 215-228		4	
2128	Measurements and prediction of VLE of methyl propanoate/ethanol/propan-1-ol at 114.6 and 127.99kPa 1990 , 23, 349-353		17	
2127	Determination of new ASOG parameters 1990 , 23, 453-463		232	
2126	VLE at 114.66 and 127.99kPa for the systems methyl acetate+ethanol and methyl acetate+propan-1-ol. Measurements and prediction 1990 , 23, 621-626		18	
2125	Dependence of solution data at ideal dilution on solvent molecular size. 1990 , 30, 493-499		7	
2124	Universal functional group activity coefficient model in electrosorption: Part I. Theory. 1990 , 135, 97-10)6		
2123	Solubility of normal alkanoic acids in selected organic binary solvent mixtures. negative synergetic effect. <i>Fluid Phase Equilibria</i> , 1990 , 58, 211-227	2.5	7	
2122	Molekulare Thermodynamik f□ 🛭 die chemische Proze 🗆 🛱 lanung. 1990 , 102, 1286-1295		3	
2121	Solubility of acetyl-substituted naphthols in binary solvent mixtures. <i>Fluid Phase Equilibria</i> , 1990 , 55, 125-145	2.5	25	
2120	A comparison of the predictive capability of different group contribution methods. <i>Fluid Phase Equilibria</i> , 1990 , 54, 147-165	2.5	29	
2119	VLE of alkanol-alkane systems with the modified CRG model. Fluid Phase Equilibria, 1990 , 56, 189-202	2.5	4	
2118	Liquid II quid equilibria for ternary systems of cyclohexane-water and butanols. Data and predictions. <i>Fluid Phase Equilibria</i> , 1990 , 57, 327-340	2.5	7	
2117	An interaction site analysis of the Bolution of groupsIfor short chain molecules. <i>Fluid Phase Equilibria</i> , 1990 , 61, 17-51	2.5	3	
2116	Prediction of compatibility in polymer-plasticizer systems. 1990 , 31, 1745-1749		7	
2115	(Liquid + liquid) equilibria of (furfural + water + ethyl ethanoate or 2-methylpropyl ethanoate or methyl benzoate or 2-ethylhexan-1-ol) at 293.15 K. 1990 , 22, 129-134		6	
2114	Excess enthalpies for (n-butyl methyl ether + n-alkane) at 298.15 K. 1990 , 22, 173-179		16	

2113	Prediction of the surface tension of binary and multicomponent liquid mixtures by the UNIFAC group contribution method. 1990 , 169, 231-238	10
2112	Prediction of phase equilibria in tributyl phosphate extraction system using the unifac group contribution method. 1990 , 169, 287-300	4
2111	Pr l'vision des propri l't l's thermodynamiques de m langes binaires contenant des alcools. 1990 , 167, 189-217	4
2110	Polycyclic Aromatic Nitrogen Heterocycles. Solubility of Carbazole in Binary Solvent Mixtures Containing Cyclohexane. 1990 , 22, 157-162	10
2109	Polycyclic Aromatic Sulfur Heterocycles. Solubility of Thianthrene in Binary Solvent Mixtures Containing Cyclohexane. 1990 , 21, 45-49	11
2108	Separating acetic acid from liquids. 1990 , 50, 51-55	7
2107	Prediction of vapourliquid equilibrium data for binary mixtures from molecular parameters using a generalized London potential. 1991 , 87, 57-62	2
2106	Prediction of the solubility of hydrophobic compounds in nonideal solvent mixtures. 1991 , 22, 939-951	22
2105	Thermochemical Investigation of Molecular Complexation: Estimation of Anthracene-ethyl Acetate and Anthracene-diethyl Adipate Association Parameters from Measured Solubility Data. 1991 , 24, 31-42	6
2104	Descriptors for isomer resolution of (bio-) distribution of chlorinated aromatic compounds. 1991 , 109-110, 105-19	4
2103	STRUCTURAL MODELS OF CATALYTIC CRACKING CHEMISTRY. 1991 , 163-180	2
2102	Fuel Methanol Composition Effects on Cold Starting. 1991,	3
2101	Polymer compatibility - a consequence of repulsive groups within monomer units. 1991 , 44, 47-59	7
2100	Vapor-Liquid Equilibria of Mixtures of Methyl Butanoate + Propan-2-ol at 74.66, 101.32, and 127.99 kPa. 1991 , 95, 1214-1219	6
2099	PSRK: A Group Contribution Equation of State Based on UNIFAC. Fluid Phase Equilibria, 1991 , 70, 251-26 5 .5	553
2098	The prediction of fluid phase equilibria of subcritical binary systems by using an equation of state. Fluid Phase Equilibria, 1991 , 64, 107-127 2.5	4
2097	Prediction of retention in gas-liquid chromatography using the UNIFAC group contribution method. 1991 , 585, 83-92	5
2096	Prediction of retention in gas-liquid chromatography using the UNIFAC group contribution method. 1991 , 586, 297-301	2

2095	(Liquid + liquid) equilibria of (ethanoic acid + an alkanol or a ketone or an ester or an aromatic hydrocarbon + water) at the temperature 293.15 K. 1991 , 23, 859-865		15
2094	Application of the UNIFAC method for assessment of retention in reversed-phase liquid chromatograhy. 1991 , 543, 267-275		5
2093	Isobaric vaporliquid equilibria for binary systems composed of methyl butanoate with ethanol and with propan-1-ol at 114.66 and 127.99 kpa. 1991 , 69, 394-397		10
2092	The solubility of hydrophobic aromatic chemicals in organic solvent/water mixtures: Evaluation of four mixed solvent solubility estimation methods. 1991 , 10, 881-889		17
2091	Infinite-dilution activity coefficients of organic solutes in methyl phenyl ether, butyl ether and methyl iso-butyl ketone. 1991 , 14, 376-378		3
2090	Thermodynamics of ammonium sulfatepolyethylene glycol aqueous two-phase systems. Part 2. Correlation and prediction using extended unifac equation. <i>Fluid Phase Equilibria</i> , 1991 , 63, 173-182	2.5	38
2089	Prediction of solid-liquid equilibria from measured adduction constants. <i>Fluid Phase Equilibria</i> , 1991 , 68, 207-218	2.5	3
2088	Empirical prediction method for activity coefficients based on 軸nd (d賴d阻0. <i>Fluid Phase Equilibria</i> , 1991 , 65, 167-179	2.5	
2087	Prediction of vapor-liquid and liquid-liquid equilibria in phenol + hydrocarbon systems. <i>Fluid Phase Equilibria</i> , 1991 , 69, 193-207	2.5	6
2086	Finding the optimum sequence of distillation columns - an equation to replace the fules of thumb[] (heuristics). 1991 , 46, 97-108		21
2085	Thermochemical investigations of associated solutions. 13. Calculation of anthracene-chlorobutane association parameters from measured solubility data. 1991 , 20, 307-318		6
2084	The predictive accuracy for estimating infinite dilution activity coefficients by b ased UNIFAC. 1991 , 20, 1189-1198		5
2083	Molecular Modelling of Micellar Solutions. 1991 , 95-111		2
2082	Applicability of the Perturbed Hard Chain Equation of State for Simulation of Distillation Processes in the Oleochemical Industry. Part I: Separation of Fatty Acids. 1992 , 27, 955-974		8
2081	Solubility of Anthracene in Binary Alkane + Dimethyl Adipate and Alkane + Dibutyl Oxalate Solvent Mixtures. 1992 , 25, 51-58		1
2080	Heat of Dilution in Aqueous and Methanolic Formaldehyde Solutions. 1992 , 96, 83-96		10
2079	Steam stripping for removal of organic pollutants from water. 2. Vapor-liquid equilibrium data. <i>Industrial & Damp; Engineering Chemistry Research</i> , 1992 , 31, 1759-1768	3.9	45
2078	An encoding system for a group contribution method. 1992 , 32, 443-447		2

2077 AQUAFAC 1: Aqueous functional group activity coefficients; application to hydrocarbons. **1992**, 24, 1047-1061 49

2076	Prediction of distribution properties by solubility parameters: Description of the method and application to methylbenzenes. 1992 , 24, 453-464		1
2075	Experimental and predicted mixing enthalpies for several methyl n-alkanoates with n-pentane at 298.15 K. 1992 , 195, 321-327		21
2074	Group unary Wilson model for liquid mixtures without arbitrary parameters. 1992 , 48, 183-190		1
2073	Vapor-liquid equilibria for binary mixtures with anisole. Fluid Phase Equilibria, 1992, 71, 85-98	2.5	30
2072	Liquid-liquid equilibria for ternary systems of cyclohexane-water and C1 to C3 alcohols: data and predictions. <i>Fluid Phase Equilibria</i> , 1992 , 71, 189-209	2.5	13
2071	A method for predicting VLE and HE of chain-like isomers using a modified UNIFAC model. <i>Fluid Phase Equilibria</i> , 1992 , 74, 47-65	2.5	2
2070	Phase equilibria in very dilute mixtures of water and unsaturated chlorinated hydrocarbons and of water and benzene. <i>Fluid Phase Equilibria</i> , 1992 , 81, 217-229	2.5	22
2069	Excess molar enthalpies of binary mixtures ethylbenzene + propylbenzene, + butylbenzene and + hexylbenzene at 298.15, 308.15 and 318.15 K. <i>Fluid Phase Equilibria</i> , 1992 , 81, 231-239	2.5	5
2068	A molecular thermodynamic approach to predict the secondary structure of homopolypeptides in aqueous systems. 1992 , 32, 1375-92		17
2067	Vaporliquid equilibria calculations with a cubic equation of state: group contributions for heavy hydrocarbons containing mixtures. 1993 , 48, 1185-1200		3
2066	Analysis of a modification of the ASOG method for vaporliquid equilibrium prediction. 1993 , 32, 277-20	81	
2065	Statistical thermodynamics of disordered and ordered systems. A properly normalized local order theory. <i>Fluid Phase Equilibria</i> , 1993 , 85, 1-18	2.5	13
2064	Liquid - liquid equilibria in hydrocarbon + 3-methoxy-propionitrile systems, correlation and prediction. <i>Fluid Phase Equilibria</i> , 1993 , 85, 161-170	2.5	5
2063	Application of equations of state and the theory of group solutions to phase equilibrium prediction. <i>Fluid Phase Equilibria</i> , 1993 , 87, 23-35	2.5	8
2062	A segment-based local composition model for the gibbs energy of polymer solutions. <i>Fluid Phase Equilibria</i> , 1993 , 83, 301-312	2.5	154
2061	The molecular interaction group contributions for dielectric solvents. <i>Fluid Phase Equilibria</i> , 1993 , 82, 389-396	2.5	1
2060	Revision of interaction parameters for estimating the enthalpies of mixtures of benzyl ethanoate + n-alkanes or 1-chloroalkanes using the UNIFAC model with presentation of new experimental data. <i>Fluid Phase Equilibria</i> , 1993 , 86, 251-273	2.5	15

2059	The solvent dependence of the solubility of organic solids and solubility parameter theory: investigation by means of an organic pigment. 1993 , 21, 273-292		7
2058	Thermodynamic properties of organic compounds. 1993 , 219, 97-104		31
2057	Application of a group-contribution method to biological systems: Prediction of water activity, ph, and related properties. 1993 , 17, S159-S164		2
2056	Heat transformation with the ternary working fluid TFE-H2O-E181. 1993 , 16, 120-128		27
2055	Lattice models for the description of partitioning/ adsorption and retention in reversed-phase liquid chromatography, including surface and shape effects. 1993 , 656, 135-196		58
2054	Quantitative structure-retention relationships applied to reversed-phase high-performance liquid chromatography. 1993 , 656, 417-435		182
2053	Study of initial- and transition-state solvation in the solvolysis of tert-butyl halides in alcohols from infinite dilution activity coefficients. 1993 , 6, 133-138		7
2052	Study of initial state and transition state solvation in the Menschutkin reaction of triethylamine with ethyl iodide in alcohols from infinite dilution activity coefficients. 1993 , 6, 595-599		5
2051	An improvement for the excess enthalpy prediction by UNIFAC. 1. Binary mixtures containing alkanes. 1993 , 22, 383-390		4
2050	Prediction of Henry's constants by the UNIFAC-FV model for hydrocarbon gases and vapors in high-boiling hydrocarbon solvents. <i>Fluid Phase Equilibria</i> , 1993 , 90, 205-217	2.5	5
2049	Vapor - liquid equilibrium of systems containing perfluoromethyl-cyclohexane and hydrocarbons. <i>Fluid Phase Equilibria</i> , 1993 , 88, 159-170	2.5	5
2048	Thermodynamics of coal-derived fluids. 1993 , 72, 1039-1045		3
2047	Estimation of the aqueous solubility of complex organic compounds. 1993 , 26, 1239-1261		43
2046	New developments of the UNIFAC model for environmental application. 1993 , 26, 1325-1354		23
2045	Extraction of Aromatic Compounds from Heavy Neutral Distillate Lubricating Oils by Using Furfural. 1993 , 28, 2465-2477		25
2044	Correlation of partition coefficients of organic solutes between water and an organic solvent. An application of the linear solvation energy relationship. <i>Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description of the linear solvation energy relationship. Industrial & Description energy relationship in the linear solvation energy relation energy relationship in the linear solvation energy relationship in the linear solvation energy relation energy relation energy relationship in the linear solvation energy relation energy relationsh</i>	3.9	23
2043	Prediction of gas solubilities in pure and mixed solvents using a group contribution method. <i>Industrial & Description of the second of the se</i>	3.9	12
2042	Simultaneous correlation of viscosity and vapor-liquid equilibrium data. <i>Industrial & amp;</i> Engineering Chemistry Research, 1993 , 32, 2077-2087	3.9	54

2041	Vapor-liquid equilibria behavior of methyl esters and propan-2-ol at 74.66, 101.32 and 127.99 kPa 1993 , 26, 259-265		13
2040	Prediction of vapor-liquid equilibrium with the LCVM model: a linear combination of the Vidal and Michelsen mixing rules coupled with the original UNIF. <i>Fluid Phase Equilibria</i> , 1994 , 92, 75-106	2.5	217
2039	Thermodynamics of potassium hydrogen phosphate- potassium dihydrogen phosphate-polyethylene glycol aqueous two-phase systems. <i>Fluid Phase Equilibria</i> , 1994 , 95, 341-357	2.5	30
2038	Measurement of water activity in water-urea-Bugarland water-urea-Bolyollsystems, and its prediction by the ASOG group contribution method. <i>Fluid Phase Equilibria</i> , 1994 , 98, 189-199	2.5	14
2037	On standard and reference states compatible with the LCVM model. <i>Fluid Phase Equilibria</i> , 1994 , 97, 53-	- 60 5	4
2036	Prediction of the solubility of aromatic hydrocarbons in supercritical CO2 with EoSGE models. <i>Fluid Phase Equilibria</i> , 1994 , 102, 121-141	2.5	25
2035	Binary interaction parameters for nonpolar systems with cubic equations of state: a theoretical approach 1. CO2/hydrocarbons using SRK equation of state. <i>Fluid Phase Equilibria</i> , 1994 , 102, 31-60	2.5	76
2034	Determination of second cross virial coefficients from gas-liquid chromatographic data. 1994 , 688, 117-	·123	1
2033	DISQUAC predictions of phase equilibria, molar and standard partial molar excess quantities for 1-alkanol+cyclohexane mixtures. 1994 , 23, 399-420		46
2032	Application of the LCVM model to multicomponent systems: Extension of the UNIFAC interaction parameter table and prediction of the phase behavior of synthetic gas condensate and oil systems. <i>Fluid Phase Equilibria</i> , 1994 , 101, 187-210	2.5	26
2031	Application of the van der Waals equation of state to polymers III. Correlation and prediction of upper critical solution temperatures for polymer solutions. <i>Fluid Phase Equilibria</i> , 1994 , 100, 63-102	2.5	23
2030	Improved models for the prediction of activity coefficients in nearly athermal mixtures: Part I. Empirical modifications of free-volume models. <i>Fluid Phase Equilibria</i> , 1994 , 92, 35-66	2.5	36
2029	Application of the van der Waals equation of state to polymers. Fluid Phase Equilibria, 1994 , 96, 93-117	2.5	26
2028	Representation of vapour-liquid equilibria in water-alcohol-electrolyte mixtures with a modified UNIFAC group-contribution method. <i>Fluid Phase Equilibria</i> , 1994 , 98, 71-89	2.5	59
2027	Phase equilibria in very dilute mixtures of water and brominated hydrocarbons. <i>Fluid Phase Equilibria</i> , 1994 , 98, 213-223	2.5	8
2026	Estimation of DISQUAC interchange energy parameters for 1-alkanols + benzene or + toluene mixtures. <i>Fluid Phase Equilibria</i> , 1994 , 93, 1-22	2.5	59
2025	Correlation and prediction of excess enthalpies of ester + n-alkane systems using the UNIFAC model. 1994 , 240, 207-213		2
2024	Determination of infinite dilution activity coefficients and second virial coefficients using gas-liquid chromatography I. the dilute mixtures of water and unsaturated chlorinated hydrocarbons and of water and benzene. 1994 , 673, 85-92		7

2023	Application of UNIFAC to vegetable oil-alkane mixtures. 1994 , 71, 391-395		23
2022	Estimation of aqueous solubility, octanol/water partition coefficient, and henry's law constant for polychlorinated biphenyls using unifac. 1994 , 29, 657-669		14
2021	DISQUAC predictions on VLE and HE for ternary mixtures containing 1-alkanols and hydrocarbons. 1994 , 98, 106-112		16
2020	Disquac application to SLE of binary mixtures containing long chain 1-alkanols (1-tetradecanol, 1-hexadecanol, 1-octadecanol, or 1-eicosanol) and N-alkanes (C8©116). 1994 , 98, 955-959		31
2019	Vapor-liquid equilibria of methyl ethanoate with n-butyl and iso-butyl alcohol at 74.66 and 127.99kPa 1995 , 28, 66-70		8
2018	Experimental and Predicted Isobaric Vapour-Liquid Equilibrium for the Binary Systems 1,2-Dibromoethane with Isomeric Butanols 1995 , 28, 721-726		3
2017	Vapor-Liquid Equilibria for Mixtures of Several Butyl Esters (Methanoate to Butanoate) and 1-Propanol at 101.32kPa 1995 , 28, 765-771		9
2016	A combinatorial activity coefficient model for symmetric and asymmetric mixtures. <i>Fluid Phase Equilibria</i> , 1995 , 109, 1-15	.5	26
2015	Measurement and correlation of liquid-liquid equilibria of methanol+alkane+ether ternary systems. Fluid Phase Equilibria, 1995 , 110, 197-204	.5	4
2014	DISQUAC predictions on excess enthalpies of the ternary mixture: cyclohexane + propanone + tetrahydrofuran. <i>Fluid Phase Equilibria</i> , 1995 , 109, 67-81	.5	7
2013	The leveling of thermosetting waterborne coatings. Part II: Drying of coated wet films. 1995 , 35, 1098-110	05	9
2012	Prediction of flux and selectivity in pervaporation through a membrane. 1995 , 107, 129-146		28
2011	A physical chemical UNIFAC model for aqueous solutions of sugars. <i>Fluid Phase Equilibria</i> , 1995 , 105, 1-25	.5	46
2010	Prediction of high-pressure vapor-liquid equilibria using ASOG. <i>Fluid Phase Equilibria</i> , 1995 , 104, 253-260 ₂	.5	17
2009	Isobaric VLE data for the binary systems dibromomethane with isomeric butanols at 40.0 and 101.3 kPa. <i>Fluid Phase Equilibria</i> , 1995 , 108, 185-198	.5	15
2008	From UNIFAC to modified UNIFAC to PSRK with the help of DDB. <i>Fluid Phase Equilibria</i> , 1995 , 107, 1-29 ₂	.5	42
2007	Application of the mobile order thermodynamics to predict the solubility of solid hydrocarbons in pure solvents and nonpolar binary solvent systems. 1995 , 67, 81-94		14
2006	Use of nuclear magnetic resonance to model thermophysical properties of frozen and unfrozen model food gels. 1995 , 25, 1-19		30

2005	Derivation of solubility parameters of chlorinated dibenzofurans and dibenzo[p]dioxins from gas chromatographic retention parameters via SOFA. 1995 , 715, 267-278		9
2004	A study of solution properties to optimize absorption cycle COP. 1995 , 18, 42-50		11
2003	Effect of water activity on enzyme hydration and enzyme reaction rate in organic solvents. 1995 , 79, 473-478		60
2002	Enzyme reaction kinetics in organic solvents: A theoretical kinetic model and comparison with experimental observations. 1995 , 79, 479-484		18
2001	Viscosity: A critical review of practical predictive and correlative methods. 1995 , 73, 3-40		152
2000	Mathematical Modeling of Adsorption Processes for the International Space Station Water Processor. 1995 ,		3
1999	A Computer-Aided Molecular Design of Fluids That Optimize Absorption Cycle COP. 1995 , 117, 156-160		4
1998	Prediction of Gas Solubilities Using the LCVM Equation of State/Excess Gibbs Energy Model. <i>Industrial & Engineering Chemistry Research</i> , 1995 , 34, 948-957	3.9	25
1997	Infinite Dilution Activity Coefficients and Solubilities of Biphenyl in Octadecane and Mineral Oil. <i>Journal of Chemical & Data</i> , 1995, 40, 746-749	2.8	7
1996	Using backpropagation networks for the estimation of aqueous activity coefficients of aromatic organic compounds. 1995 , 35, 723-8		31
1995	Solubility of Hydrogen, Carbon Monoxide, and 1-Octene in Various Solvents and Solvent Mixtures. Journal of Chemical & Engineering Data, 1996, 41, 1414-1417	2.8	107
1994	Physical, Chemical, and Microbiological Characteristics of Dehydrated Foods. 1996 , 29-99		7
1993	A Simplified Perturbed Hard-Sphere Model for the Activity Coefficients of Amino Acids and Peptides in Aqueous Solutions. <i>Industrial & Engineering Chemistry Research</i> , 1996 , 35, 4319-4327	3.9	63
1992	Liquidliquid Equilibria of the Ternary System Water + Acetic Acid + 2-Methyl-2-butanol. <i>Journal of Chemical & Engineering Data</i> , 1996 , 41, 1311-1314	2.8	26
1991	Pervaporation: Principles and Applications. 1996 , 25, 131-224		25
1990	Viscometric Study of (an Aliphatic Methyl Ester + Heptane or Nonane) at the Temperature 298.15 K. Journal of Chemical &	2.8	25
1989	Solvent Effects in the Carbonylation of Methanol. <i>Industrial & Engineering Chemistry Research</i> , 1996 , 35, 3044-3054	3.9	6
1988	Densities and Isobaric Vapor[liquid Equilibria for the Mixtures Formed by Four Butyl Esters and 1-Butanol. <i>Journal of Chemical & Engineering Data</i> , 1996 , 41, 53-58	2.8	34

1987	Phase Equilibria of the Ternary System Water + Acetic Acid + 1-Pentanol. <i>Journal of Chemical & Engineering Data</i> , 1996 , 41, 562-565	2.8	15
1986	A Perturbed Hard-Sphere Model with Mean Spherical Approximation for the Activity Coefficients of Amino Acids in Aqueous Electrolyte Solutions. <i>Industrial & Discourse Engineering Chemistry Research</i> , 1996 , 35, 4755-4766	3.9	27
1985	A critical review of Henry's law constants for environmental applications. 1996 , 26, 205-297		227
1984	Densities and Vaporliquid Equilibria in Binary Mixtures Formed by Propyl Methanoate + Ethanol, +Propan-1-ol, and +Butan-1-ol at 160.0 kPall Journal of Chemical & Engineering Data, 1996, 41, 859-8	3 6 4 ⁸	10
1983	Prediction of Infinite-Dilution Activity Coefficients in Binary Mixtures with UNIFAC. A Critical Evaluation. <i>Industrial & Evaluation amp; Engineering Chemistry Research</i> , 1996 , 35, 1438-1445	3.9	53
1982	Infinite Dilution Activity Coefficients Predicted from UNIFAC Model. New Experimental Data for the Solvolytic Reactions of 2-Chloro-2-methylpropane in Methanol/Ethanol, Methanol/2-Methoxyethanol, and Ethanol/2-Methoxyethanol. <i>Industrial & Data Communication of the Communication of</i>	3.9	2
1981	UNIFAC Prediction of Aqueous and Nonaqueous Solubilities of Chemicals with Environmental Interest. 1996 , 30, 1369-1376		48
1980	Linear Solvation Energy Relationship of the Limiting Partition Coefficient of Organic Solutes between Water and Activated Carbon. 1996 , 30, 143-152		69
1979	Prediction of Vaporlliquid Equilibria of Associating Mixtures with UNIFAC Models That Include Association. <i>Industrial & Engineering Chemistry Research</i> , 1996 , 35, 4656-4666	3.9	14
1978	Estimating water solubilities of organics as a function of temperature. 1996 , 30, 2222-2225		11
1977	Acyl Group Migrations in 2-Monoolein. 1996 , 14, 89-111		88
1976	Thermal-Hydraulic Modeling of Supercritical Water Oxidation of Ethanol. 1996 , 10, 326-332		40
1975	Measurements and analysis of excess volumes of some alkan-2-one-1-chloroalkane mixtures using Nitta©hao and PrigogineEloryPatterson models. 1996 , 92, 4453-4461		11
1974	Development of a Universal Group Contribution Model for Single-Component and Multicomponent Adsorption of Liquids on Various Adsorbents (UGCMA). <i>Industrial & Description of Liquids on Various Adsorbents (UGCMA)</i> . <i>Industrial & Description of Liquids on Various Adsorbents (UGCMA)</i> . <i>Industrial & Description of Liquids on Various Adsorbents (UGCMA)</i> . <i>Industrial & Description of Liquids (UGCMA)</i> .	3.9	8
1973	Vapour-Liquid Equilibrium of the Ternary System (Benzene + Cyclohexane + Hexane) at 40.0 kPa AND 101.3 kPa. 1996 , 31, 21-31		3
1972	Mixing rules for accurate prediction of vapor-liquid equilibria of gas/large alkane systems using SRK equation of state combined with unifac 1996 , 29, 315-322		20
1971	A new mixing rule for accurate prediction of high pressure vapor-liquid equilibria of Gas/Large n-alkane systems. 1996 , 12, 235-240		
1970	Predictive quasilattice equation of state for unified high pressure phase equilibria of pure fluids and mixtures. 1996 , 12, 385-388		1

1969	Vapor-liquid equilibria at 101.32kPa mixtures of butyl esters and propan-2-ol 1996 , 29, 294-299		9
1968	A new lattice-fluid equation of state and its group contribution applications for predicting phase equilibria of mixtures. <i>Fluid Phase Equilibria</i> , 1996 , 117, 48-54	2.5	20
1967	Thermodynamics of coal-derived fluids. 3. VLE and heat capacities of coal liquid fractions. 1996 , 75, 363	-372	
1966	Threshold chemosensitivity and hypothetical chemoreceptor function of the nematodeCaenorhabditis elegans. 1996 , 22, 1463-75		2
1965	Kondensation von Dampfgemischen Teil 3. 1996 , 62, 81-89		2
1964	Solvent activity coefficients at infinite dilution in polystyrene-hydrocarbon systems from inverse gas chromatography. 1996 , 13, 129-135		6
1963	Evaluation of a model for the prediction of phase equilibria from general molecular parameters II: Binary liquid-liquid equilibria at low pressures. 1996 , 51, 141-148		1
1962	Evaluation of a model for the prediction of phase equilibria from general molecular parameters I: Vapour-liquid equilibria and enthalpy at low pressures. 1996 , 51, 127-140		2
1961	Group-contribution theory for adsorption of gas mixtures on solid surfaces. 1996 , 51, 4025-4038		17
1960	Prediction of enthalpies of mixing and vapor-liquid equilibria for mixtures containing organic carbonates + n-alkanes using several versions of the unifac model. 1996 , 286, 321-332		20
1959	Rapid plant-wide screening of solvents for batch processes. 1996 , 20, S375-S380		11
1958	UNIFAC activity coefficient derivatives. 1996 , 10, 177-180		1
1957	The analysis of sorption data of organic vapors in polymeric membranes through novel theories. 1996 , 113, 57-64		17
1956	A comparison of lattice-fluid models for the calculation of the liquid-liquid equilibria of polymer solutions. <i>Fluid Phase Equilibria</i> , 1996 , 114, 47-62	2.5	13
1955	Isobaric vapor-liquid equilibria for methyl esters + butan-2-ol at different pressures. <i>Fluid Phase Equilibria</i> , 1996 , 118, 249-270	2.5	12
1954	Water solubilities in blends of gasoline and oxygenates. Fluid Phase Equilibria, 1996, 116, 437-444	2.5	25
1953	Application of the group-contribution lattice-fluid equation of state to random copolymer-solvent systems. <i>Fluid Phase Equilibria</i> , 1996 , 117, 33-39	2.5	23
1952	A review of practical calculation methods for the viscosity of liquid hydrocarbons and their mixtures. <i>Fluid Phase Equilibria</i> , 1996 , 117, 344-355	2.5	108

1951	Solubility of anthracene and anthraquinone in acetonitrile, methyl ethyl ketone, isopropol alcohol and their mixtures. <i>Fluid Phase Equilibria</i> , 1996 , 121, 267-272	2.5	14	
1950	Experimental study of miscibility, density and isobaric vapor-liquid equilibrium values for mixtures of methanol in hydrocarbons (C5, C6). <i>Fluid Phase Equilibria</i> , 1996 , 122, 207-222	2.5	24	
1949	Revisionist look at solvophobic driving forces in reversed-phase liquid chromatography III. Comparison of the behavior of nonpolar and polar solutes. 1996 , 724, 1-12		42	
1948	Delayed adsorption on slowly accessible stationary phase surfaces in porous liquid chromatographic column packings. 1996 , 728, 97-112		2	
1947	Application of the LCVM model to systems containing organic compounds and supercritical carbon dioxide. 1996 , 9, 88-98		33	
1946	Vapor-liquid equilibria at 101.32 kPa in mixtures formed by the first four butyl alkanoates and butan-2-ol. <i>Fluid Phase Equilibria</i> , 1996 , 124, 161-175	2.5	11	
1945	A new predictive quasi-lattice equation of state for high-pressure phase equilibria of pure fluids and mixtures. <i>Fluid Phase Equilibria</i> , 1996 , 125, 21-31	2.5	5	
1944	Phase equilibria of the ternary system water/acetic acid/2-pentanol. <i>Fluid Phase Equilibria</i> , 1996 , 123, 189-203	2.5	25	
1943	Generation of microcellular polyurethane foams via polymerization in carbon dioxide. I: Phase behavior of polyurethane precursors. 1996 , 36, 2404-2416		22	
1942	Measurements of Solubilities of Two Amino Acids in Water and Prediction by the UNIFAC Model. 1996 , 12, 371-379		38	
1941	Viscosities of the ternary mixture (1-butanol + n-hexane + 1-butylamine) at the temperatures 298.15 and 313.15 K. <i>Fluid Phase Equilibria</i> , 1996 , 124, 147-159	2.5	35	
1940	Dye solubility. 1996 , 145-195		5	
1939	Supercritical fluid extraction and its application in the food industry. 1996 , 17-64		7	
1938	Prediction of the vapour-liquid coexistence curve of alkanols by molecular simulation. 1996 , 87, 87-101		34	
1937	Influence of Water Activity and Support Material on the Enzymatic Synthesis of a Cck-8 Tripeptide Fragment. 1996 , 13, 165-178		14	
1936	Effectiveness of Chemically Enhanced Solubilization of Hydrocarbons. 1997 , 12, 153-158		1	
1935	Vapor-liquid equilibria calculation in gas/large alkane systems using group contribution equation of state 1997 , 30, 1133-1137		2	
1934	Phase Equilibria of the Ternary System Water + Propionic Acid + 2-Butanol. 1997 , 32, 1463-1476		13	

1933	Unified Description of Real Fluids and Their Mixtures by Group-Contribution Lattice-Hole Theory. 1997 , 101, 1072-1076	7
1932	Locating All Homogeneous Azeotropes in Multicomponent Mixtures. <i>Industrial & amp; Engineering Chemistry Research</i> , 1997 , 36, 160-178	53
1931	Method for Estimating Critical Properties of Heavy Compounds Suitable for Cubic Equations of State and Its Application to the Prediction of Vapor Pressures. <i>Industrial & Engineering State Research</i> , 1997 , 36, 4008-4012	14
1930	Analysis of the UNIFAC-Type Group-Contribution Models at the Highly Dilute Region. 1. Limitations of the Combinatorial and Residual Expressions. <i>Industrial & Empirical & Industrial & Ind</i>	21
1929	Modeling of LiquidIliquid Equilibrium and Mass Transfer. Suspension Copolymerization of Acrylic Acid and Methyl Methacrylate in Water. <i>Industrial & Engineering Chemistry Research</i> , 1997 , 36, 4815-4820	O
1928	Extraction of Aromatics from Petroleum Naphtha Reformate by a 1-Cyclohexyl-2-pyrrolidone/Ethylene Carbonate Mixed Solvent. <i>Industrial & amp; Engineering</i> 3.9 <i>Chemistry Research</i> , 1997 , 36, 414-418	13
1927	Water Absorption by Organics: Survey of Laboratory Evidence and Evaluation of UNIFAC for Estimating Water Activity. 1997 , 31, 3318-3324	100
1926	A Thermodynamic Approach Using Group Contribution Methods to Model the Partitioning of Semivolatile Organic Compounds on Atmospheric Particulate Matter. 1997 , 31, 2805-2811	107
1925	Vaporliquid Equilibria and Densities for Ethyl Esters (Ethanoate to Butanoate) and Alkan-2-ol (C3\(\text{C4}\)) at 101.32 kPa. Journal of Chemical & amp; Engineering Data, 1997 , 42, 1090-1100	34
1924	Gas/Particle Partitioning of Semivolatile Organic Compounds To Model Inorganic, Organic, and Ambient Smog Aerosols. 1997 , 31, 3086-3092	134
1923	Liquid Diquid Equilibria of the Ternary System Water + Acetic Acid + 1-Hexanol. <i>Journal of Chemical & Engineering Data</i> , 1997 , 42, 183-186	55
1922	Measurement and Prediction of Ternary Solid[liquid Equilibria. <i>Journal of Chemical & Data, 1997, 42, 886-889</i> 2.8	7
1921	Vapor Pressure Equations for Characterizing Automotive Fuel Behavior Under Hot Fuel Handling Conditions. 1997 ,	6
1920	A new GE-mixing-rule using the Dohrn-Prausnitz equation of state for the prediction of phase equilibria of nonideal mixtures. <i>Fluid Phase Equilibria</i> , 1997 , 131, 37-49	4
1919	A conjugation-based version of the UNIFAC method. <i>Fluid Phase Equilibria</i> , 1997 , 137, 111-119 2.5	
1918	A refined latticeBole theory with group contribution for unified description of single- and multi-component real fluids. <i>Fluid Phase Equilibria</i> , 1997 , 136, 49-62	4
1917	A modified UNIFAC model for the calculation of thermodynamic properties of aqueous and non-aqueous solutions containing sugars. <i>Fluid Phase Equilibria</i> , 1997 , 139, 47-74	66
1916	Simulation of Heterogeneous Azeotropic Distillation. 1997 , 75, 101-115	12

1915	GEQUAC, an excess Gibbs energy model for simultaneous description of associating and non-associating liquid mixtures. 1997 , 101, 209-218		10
1914	Liquid phase methanol synthesis from CO2 utilizing liquid-liquid separation. 1997 , 36, 33-37		2
1913	A group contribution model for thermodynamic and transport properties of dilute gases. <i>Fluid Phase Equilibria</i> , 1997 , 129, 69-88	2.5	11
1912	Measurement and prediction of water activity in electrolyte solutions by a modified ASOG group contribution method. <i>Fluid Phase Equilibria</i> , 1997 , 129, 267-283	2.5	26
1911	Estimation of parameters of Nitta-Chao model for linear monoether + 1-alkanol mixtures. <i>Fluid Phase Equilibria</i> , 1997 , 133, 57-72	2.5	13
1910	A generalized expression for the ratio of the critical temperature to the critical pressure with the van der Waals surface area. <i>Fluid Phase Equilibria</i> , 1997 , 140, 145-156	2.5	11
1909	Prediction of phase equilibria in hydrocarbon + near-critical solvent systems. <i>Fluid Phase Equilibria</i> , 1997 , 140, 73-85	2.5	9
1908	An EOS/GE type mixing rule for perturbed hard-sphere equation of state and its application to the calculation of solid solubility in supercritical carbon dioxide. <i>Fluid Phase Equilibria</i> , 1997 , 141, 13-23	2.5	13
1907	Infinite dilution activity coefficients of apple juice aroma compounds. 1997, 34, 145-158		40
1906	An activity coefficient model for proteins. 1997 , 55, 65-71		15
1906 1905	An activity coefficient model for proteins. 1997, 55, 65-71 Prediction of water adsorption curves for heterogeneous biocatalysis in organic and supercritical solvents. 1997, 52, 213-220		15 32
1905	Prediction of water adsorption curves for heterogeneous biocatalysis in organic and supercritical		
1905	Prediction of water adsorption curves for heterogeneous biocatalysis in organic and supercritical solvents. 1997 , 52, 213-220 AZEOPERT: An expert system for the prediction of azeotrope formation Binary azeotropes.		32
1905 1904 1903	Prediction of water adsorption curves for heterogeneous biocatalysis in organic and supercritical solvents. 1997, 52, 213-220 AZEOPERT: An expert system for the prediction of azeotrope formation Binary azeotropes. 1997, 21, 93-111 Application of Different Group Contribution Models and Empirical Methods to Excess Enthalpies of		32
1905 1904 1903	Prediction of water adsorption curves for heterogeneous biocatalysis in organic and supercritical solvents. 1997, 52, 213-220 AZEOPERT: An expert system for the prediction of azeotrope formation Binary azeotropes. 1997, 21, 93-111 Application of Different Group Contribution Models and Empirical Methods to Excess Enthalpies of Ternary Mixtures. 1998, 52, 799-814		32 4 10
1905 1904 1903	Prediction of water adsorption curves for heterogeneous biocatalysis in organic and supercritical solvents. 1997, 52, 213-220 AZEOPERT: An expert system for the prediction of azeotrope formation Binary azeotropes. 1997, 21, 93-111 Application of Different Group Contribution Models and Empirical Methods to Excess Enthalpies of Ternary Mixtures. 1998, 52, 799-814 Simultaneous Synthesis of Mass Separating Agents and Interception Networks. 1998, 76, 376-388	2.5	32 4 10 21
1905 1904 1903 1902	Prediction of water adsorption curves for heterogeneous biocatalysis in organic and supercritical solvents. 1997, 52, 213-220 AZEOPERT: An expert system for the prediction of azeotrope formation Binary azeotropes. 1997, 21, 93-111 Application of Different Group Contribution Models and Empirical Methods to Excess Enthalpies of Ternary Mixtures. 1998, 52, 799-814 Simultaneous Synthesis of Mass Separating Agents and Interception Networks. 1998, 76, 376-388 Modified UNIFAC parameters for mixtures with isocyanates. 1998, 53, 2395-2401 The effects of selected solvents on the relative volatility of a binary system consisting of 1-octene	2.5	32 4 10 21

1897	Excess enthalpy and vaporliquid equilibrium prediction using non-random lattice fluid equation of state. <i>Fluid Phase Equilibria</i> , 1998 , 150-151, 199-206	2.5	7
1896	Contaminant transport resulting from multicomponent nonaqueous phase liquid pool dissolution in three-dimensional subsurface formations. 1998 , 31, 1-21		42
1895	Modeling the partitioning of BTEX in water-reformulated gasoline systems containing ethanol. 1998 , 34, 315-341		56
1894	Liquid []quid equilibria of ternary ETBE-ETOH-H2O and quaternary ETBE-ETOH-H2O-TBA mixtures. 1998 , 76, 828-831		10
1893	Oxidation of hydrocarbons by hydrogen peroxide over Ti catalysts: Kinetics and mechanistic studies. 1998 , 76, 833-852		20
1892	Kinetics of 2-hexanol and 3-hexanol oxidation reaction over TS-1 catalysts. <i>AICHE Journal</i> , 1998 , 44, 1438	₃ .16454	110
1891	Revision and Extension of the Group Contribution Method Modified UNIFAC (Dortmund). 1998 , 21, 245-2	248	15
1890	Characterization of Porous Media by Digital Image Processing. 1998 , 21, 248-253		2
1889	Kinetic and thermodynamic study of 2-bromo-2-methylbutane, 2-chloro-2-methylbutane and 3-chloro-3-methylpentane in diols. 1998 , 11, 36-40		2
1888	Design of chemical compounds. 1998 , 22, 713-715		9
1888	Design of chemical compounds. 1998, 22, 713-715 Use of evolutionary algorithms for the calculation of group contribution parameters in order to predict thermodynamic properties. Part 1: Genetic algorithms. 1998, 22, 1559-1572		9
	Use of evolutionary algorithms for the calculation of group contribution parameters in order to		
1887	Use of evolutionary algorithms for the calculation of group contribution parameters in order to predict thermodynamic properties. Part 1: Genetic algorithms. 1998 , 22, 1559-1572 Thermodynamic properties of n-alkylbenzene+n-alkane or cyclohexane mixtures. Comparison with disquac predictions. 1998 , 311, 1-19 Application of UNIFAC models to partition coefficients of biochemicals between water and	2.5	6
1887	Use of evolutionary algorithms for the calculation of group contribution parameters in order to predict thermodynamic properties. Part 1: Genetic algorithms. 1998, 22, 1559-1572 Thermodynamic properties of n-alkylbenzene+n-alkane or cyclohexane mixtures. Comparison with disquac predictions. 1998, 311, 1-19 Application of UNIFAC models to partition coefficients of biochemicals between water and n-octanol or n-butanol. <i>Fluid Phase Equilibria</i> , 1998, 144, 87-95 Prediction of infinite dilution activity coefficients in aqueous solutions by group contribution	2.5 2.5	6
1887 1886 1885	Use of evolutionary algorithms for the calculation of group contribution parameters in order to predict thermodynamic properties. Part 1: Genetic algorithms. 1998, 22, 1559-1572 Thermodynamic properties of n-alkylbenzene+n-alkane or cyclohexane mixtures. Comparison with disquac predictions. 1998, 311, 1-19 Application of UNIFAC models to partition coefficients of biochemicals between water and n-octanol or n-butanol. <i>Fluid Phase Equilibria</i> , 1998, 144, 87-95 Prediction of infinite dilution activity coefficients in aqueous solutions by group contribution models. A critical evaluation. <i>Fluid Phase Equilibria</i> , 1998, 144, 97-112		6 36 8
1887 1886 1885 1884	Use of evolutionary algorithms for the calculation of group contribution parameters in order to predict thermodynamic properties. Part 1: Genetic algorithms. 1998, 22, 1559-1572 Thermodynamic properties of n-alkylbenzene+n-alkane or cyclohexane mixtures. Comparison with disquac predictions. 1998, 311, 1-19 Application of UNIFAC models to partition coefficients of biochemicals between water and n-octanol or n-butanol. Fluid Phase Equilibria, 1998, 144, 87-95 Prediction of infinite dilution activity coefficients in aqueous solutions by group contribution models. A critical evaluation. Fluid Phase Equilibria, 1998, 144, 97-112 A completely normalized quasi-chemical theory. Fluid Phase Equilibria, 1998, 145, 217-224 Experimental VLE at 101.32 kPa in binary systems composed of ethyl methanoate and alkan-1-ols	2.5	6 36 8 30
1887 1886 1885 1884	Use of evolutionary algorithms for the calculation of group contribution parameters in order to predict thermodynamic properties. Part 1: Genetic algorithms. 1998, 22, 1559-1572 Thermodynamic properties of n-alkylbenzene+n-alkane or cyclohexane mixtures. Comparison with disquac predictions. 1998, 311, 1-19 Application of UNIFAC models to partition coefficients of biochemicals between water and n-octanol or n-butanol. <i>Fluid Phase Equilibria</i> , 1998, 144, 87-95 Prediction of infinite dilution activity coefficients in aqueous solutions by group contribution models. A critical evaluation. <i>Fluid Phase Equilibria</i> , 1998, 144, 97-112 A completely normalized quasi-chemical theory. <i>Fluid Phase Equilibria</i> , 1998, 145, 217-224 Experimental VLE at 101.32 kPa in binary systems composed of ethyl methanoate and alkan-1-ols or alkan-2-ols and treatment of data using a correlation with temperature-dependent parameters. <i>Fluid Phase Equilibria</i> , 1998, 146, 351-370 Prediction of infinite dilution activity coefficients for systems including water based on the group	2.5 2.5	6 36 8 30 7

1879	Viscosities of the ternary mixture (1-butanol+n-hexane+1-chlorobutane) at 298.15 K and 313.15 K. <i>Fluid Phase Equilibria</i> , 1998 , 152, 133-148	2.5	25	
1878	Studies on UNIQUAC and SAFT equations for nonionic surfactant solutions. <i>Fluid Phase Equilibria</i> , 1998 , 153, 215-229	2.5	25	
1877	Separation of Close-Boiling Mixtures of 4-Methoxyphenol/Catechol with tert-Butanol. 1998, 33, 1511-1	528	3	
1876	A Thermodynamic Approach for Modeling Partitioning of Semivolatile Organic Compounds on Atmospheric Particulate Matter: Humidity Effects. 1998 , 32, 1237-1243		83	
1875	Molecular Thermodynamics in the Design of Substitute Solvents. <i>Industrial & Design of Substitute Solvents</i> .	3.9	17	
1874	Measurement and Prediction of Reid Vapor Pressure of Gasoline in the Presence of Additives. <i>Journal of Chemical & Data, 1998, 43, 386-392</i>	2.8	31	
1873	High-Pressure VaporLiquid and SolidLas Equilibria Using a PengRobinson Group Contribution Method. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 3731-3740	3.9	18	
1872	Prediction of Infinite Dilution Activity Coefficients of Organic Compounds in Aqueous Solution from Molecular Structure. 1998 , 38, 200-209		30	
1871	A Modified UNIFAC (Dortmund) Model. 3. Revision and Extension. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 4876-4882	3.9	273	
1870	Liquid[liquid Equilibria of Systems Containing Propylene Carbonate and Some Hydrocarbons. <i>Journal of Chemical & Data, 1998, 43, 884-888</i>	2.8	12	
1869	Isobaric Vaporlliquid Equilibria for Ternary Mixtures: Saturated Hydrocarbons, Xylenes, and Ethylbenzene with Sulfolane at 101.325 kPa. <i>Journal of Chemical & Engineering Data</i> , 1998 , 43, 396	- 39 9	4	
1868	Synthesis of Distillation Processes Using Thermodynamic Models and the Dortmund Data Bank. <i>Industrial & Engineering Chemistry Research</i> , 1998 , 37, 3112-3123	3.9	95	
1867	Prediction of octanol-water partition coefficients, Henry coefficients and water solubilities using UNIFAC. 1998 , 65, 57-86		40	
1866	USING THE GROUP-INTERACTION CONTRIBUTION APPROACH (GIC) IN MIXTURES 1. Prediction of Azeotropic Parameters. 1998 , 169, 1-23		2	
1865	Mass transfer properties of osmotic solutions. I. Water activity and osmotic pressure. 1998 , 1, 95-112		22	
1864	Correlation and prediction of liquid phase adsorption equilibria. 1998 , 48-51		1	
1863	Encapsulated Evolution strategies for the determination of group contribution model parameters in order to predict thermodynamic properties. 1998 , 978-987		2	
1862	Macroscopic Model of the D86 Fuel Volatility Procedure. 1998 ,		15	

1861	Solvent replacement for green processing. 1998 , 106 Suppl 1, 253-71	63
1860	Modeling the chemistry of complex petroleum mixtures. 1998 , 106 Suppl 6, 1441-8	56
1859	Vapor and Liquid Composition Differences Resulting from Fuel Evaporation. 1999,	1
1858	Liquid-Liquid Equilibria, and Thermodynamic Properties of the System Methyl Acetate + Methanol + Water at 298.15 K. 1999 , 37, 193-213	16
1857	Modeling and prediction of pH and water activity in aqueous amino acid solutions. 1999 , 23, S383-S386	4
1856	Water activity in poly(ethylene glycol) aqueous solutions. 1999 , 328, 169-176	116
1855	Temperature dependence of excess molar volumes in (n-alkane (C6©9) or alcohol (C2©4))+olive oil mixtures. 1999 , 328, 277-296	50
1854	Molar excess enthalpies of binary mixtures of the three glycols ethanediol, 1,2-propanediol and 1,2-butanediol with methanol or ethanol. 1999 , 337, 209-217	12
1853	Contributions of additional group interaction parameters through limiting activity coefficient measurements on aliphatic alcohols, aromatic hydrocarbons, ketones and an ester in organic phosphates1IICT Communication No. 3864.1. 1999 , 72, 31-36	1
1852	Contributions of additional group interaction parameters through limiting activity coefficient measurements on aliphatic alcohols, aromatic hydrocarbons, ketones and an ester in tetrahydroxyethylethylenediamine and tetraethylene pentamine. 1999 , 75, 87-92	2
1851	Proximity effects and cyclization in oxaalkanes+CCl4 mixtures DISQUAC characterization of the ClD interactions. Comparison with Dortmund UNIFAC results. <i>Fluid Phase Equilibria</i> , 1999 , 154, 11-31	36
1850	Thermophysical properties of methanol+some polyethylene glycol dimethyl ether by UNIFAC and DISQUAC group-contribution models for absorption heat pumps. <i>Fluid Phase Equilibria</i> , 1999 , 155, 327-337	13
1849	Refrigeration with electrolytic and immiscible liquid I quid systems. Fluid Phase Equilibria, 1999, 158-160, 401-409	3
1848	Prediction of thermodynamic properties using a modified UNIFAC model: application to sugar industrial systems. <i>Fluid Phase Equilibria</i> , 1999 , 158-160, 391-399	12
1847	GEQUAC, an excess Gibbs energy model describing associating and nonassociating liquid mixtures by a new model concept for functional groups. <i>Fluid Phase Equilibria</i> , 1999 , 158-160, 381-389	12
1846	Activity coefficients of associating mixtures by group contribution. Fluid Phase Equilibria, 1999, 163, 195-297	42
1845	A new method for the prediction of VLE and thermodynamic properties. Preliminary results with alkane@ther@lkanol systems. <i>Fluid Phase Equilibria</i> , 1999 , 156, 35-50	10
1844	A phase stability analysis of the combinatorial term of the UNIQUAC model. 1999 , 54, 893-896	5

1843	USE of UNIFAC IN the PREDICTION of WATER ACTIVITY VALUES of AQUEOUS POLYOL SOLUTIONS. 1999 , 23, 109-120	3
1842	Thermodynamic prediction of active ingredient loading in polymeric microparticles. 1999 , 60, 77-100	22
1841	Optimal design of solvent blends for environmental impact minimization. <i>AICHE Journal</i> , 1999 , 45, 817-8 48	83
1840	Infinite dilution activity coefficients from ab initio solvation calculations. <i>AICHE Journal</i> , 1999 , 45, 2606-2 6 08	56
1839	Prediction of Vapor-Liquid Equilibria Using Peng-Robinson and Soave-Redlich-Kwong Equations of State. 1999 , 22, 379-399	31
1838	Protein solubility modeling. 1999 , 64, 144-50	19
1837	Prediction of Octanol Water Partition Coefficients Using a Group Contribution Solvation Model. Industrial & Chemistry Research, 1999, 38, 4081-4091 3-9	47
1836	Experimental and Theoretical Study of Excess Molar Enthalpies of Ethyl Propionate + n-Hexane + 1-Butanol at 298.15 K. <i>Journal of Chemical & Engineering Data</i> , 1999 , 44, 860-864	5
1835	Assessment of Activity Coefficient Models for Predicting Solidliquid Equilibria of Asymmetric Binary Alkane Systems. <i>Industrial & Engineering Chemistry Research</i> , 1999 , 38, 316-323	19
1834	Correlation and Prediction of Liquid-Phase Adsorption on Zeolites Using Group Contributions Based on AdsorbateBolid Solution Theory 1999, 15, 6035-6042	12
1833	Comparative Study of Semitheoretical Models for Predicting Infinite Dilution Activity Coefficients of Alkanes in Organic Solvents. <i>Industrial & Engineering Chemistry Research</i> , 1999 , 38, 4104-4109	28
1832	Molecular Structure Disassembly Program (MOSDAP): A Chemical Information Model To Automate Structure-Based Physical Property Estimation. 1999 , 39, 463-474	7
1831	Improved Recovery of an Ester Flavor Compound by Pervaporation Coupled with a Flash Condensation. <i>Industrial & Description Compound Strong Chemistry Research</i> , 1999 , 38, 4458-4469	28
1830	Estimation of Physical Properties. 2000,	1
1829	Computer-Aided Engineering (CAE). 2000,	
1828	A continuous polydisperse thermodynamic algorithm for a modified floryHuggins model: The (polystyrene + nitroethane) example. 2000 , 38, 632-651	34
1827	Predictive models for the viscosities of multicomponent liquid n-Alkane and regular solutions. 2000 , 78, 355-362	8
1826	Solubilities of anthracene, fluoranthene and pyrene in organic solvents: Comparison of calculated values using UNIFAC and modified UNIFAC (Dortmund) models with experimental data and values using the mobile order theory 2000 , 78, 1168-1174	30

1825	On the development of novel chemicals using a systematic synthesis approach. Part I. Optimisation framework. 2000 , 55, 2529-2546	64
1824	Prediction of the viscosity of multi-component liquid mixtures:. 2000 , 55, 2861-2873	23
1823	Solid substrate cultivation of Gibberella fujikuroi on an inert support. 2000 , 35, 1227-1233	31
1822	Kinetic of liquid-phase reactions catalyzed by acidic resins: the formation of peracetic acid for vegetable oil epoxidation. 2000 , 197, 165-173	47
1821	Revision and extension of the group contribution equation of state to new solvent groups and higher molecular weight alkanes. <i>Fluid Phase Equilibria</i> , 2000 , 172, 129-143	40
1820	A group contribution correlation of the mutual diffusion coefficients of binary liquid mixtures. <i>Fluid Phase Equilibria</i> , 2000 , 173, 1-21	21
1819	Isobaric vaporlīquid equilibria of alkyl carbonates with alcohols. Fluid Phase Equilibria, 2000 , 175, 91-105 2.5	61
1818	Thermodynamics of mixtures with strongly negative deviations from Raoult's Law. <i>Fluid Phase Equilibria</i> , 2000 , 168, 31-58	133
1817	Measurements and model prediction of the solid I quid equilibria of organic binary mixtures. 2000 , 55, 3175-3185	52
	Consolibility Doors to Delivera Michigan Associated by the color of the consolir of the color of	
1816	Compatibility Range in Polymer Mixtures. An approach using analogue calorimetry and group contribution procedures. 2000 , 62, 135-151	4
1816 1815		
1815	Contribution procedures. 2000 , 62, 135-151 Kinetics of Catalytic Esterification of Acetic Acid and Amyl Alcohol over Dowex. <i>Industrial & Esterification of Acetic Acid and Amyl Alcohol over Dowex</i> . <i>Industrial & Esterification of Acetic Acid and Amyl Alcohol over Dowex</i> .	-
1815	Contribution procedures. 2000, 62, 135-151 Kinetics of Catalytic Esterification of Acetic Acid and Amyl Alcohol over Dowex. <i>Industrial & Engineering Chemistry Research</i> , 2000, 39, 4094-4099	108
1815 1814	Contribution procedures. 2000, 62, 135-151 Kinetics of Catalytic Esterification of Acetic Acid and Amyl Alcohol over Dowex. <i>Industrial & Engineering Chemistry Research</i> , 2000, 39, 4094-4099 Viscosity prediction for fatty systems. 2000, 77, 1255-1262 Swelling equilibria of polymeric hydrogels containing poly(acrylamidesodiumallylsulfonate-acrylic	108 59
1815 1814 1813	Kinetics of Catalytic Esterification of Acetic Acid and Amyl Alcohol over Dowex. <i>Industrial & Engineering Chemistry Research</i> , 2000 , 39, 4094-4099 Viscosity prediction for fatty systems. 2000 , 77, 1255-1262 Swelling equilibria of polymeric hydrogels containing poly(acrylamidesodiumallylsulfonate-acrylic acid). 2000 , 17, 534-540 Prediction of Water Activity in Sugar Solutions Using Models of Group Contribution and Equation of	108 59 7 23
1815 1814 1813 1812	Contribution procedures. 2000, 62, 135-151 Kinetics of Catalytic Esterification of Acetic Acid and Amyl Alcohol over Dowex. <i>Industrial & Samp; Engineering Chemistry Research</i> , 2000, 39, 4094-4099 Viscosity prediction for fatty systems. 2000, 77, 1255-1262 Swelling equilibria of polymeric hydrogels containing poly(acrylamidesodiumallylsulfonate-acrylic acid). 2000, 17, 534-540 Prediction of Water Activity in Sugar Solutions Using Models of Group Contribution and Equation of State 2000, 33, 645-653 Enzymatic Production of Alkyl Esters Through Lipase-Catalyzed Transesterification Reactions in	108 59 7 23
1815 1814 1813 1812	Kinetics of Catalytic Esterification of Acetic Acid and Amyl Alcohol over Dowex. <i>Industrial & Engineering Chemistry Research</i> , 2000 , 39, 4094-4099 Viscosity prediction for fatty systems. 2000 , 77, 1255-1262 Swelling equilibria of polymeric hydrogels containing poly(acrylamidesodiumallylsulfonate-acrylic acid). 2000 , 17, 534-540 Prediction of Water Activity in Sugar Solutions Using Models of Group Contribution and Equation of State 2000 , 33, 645-653 Enzymatic Production of Alkyl Esters Through Lipase-Catalyzed Transesterification Reactions in Organic Solvents: Solvent Effects and Prediction Capabilities of Equilibrium Conversions. 2000 , 18, 259-269	108 59 7 23 4

(2001-2000)

1807	Liquid Diquid Equilibria of Acetone + Methanol + n-Alkane (C6 128) at Different Temperatures. Journal of Chemical & Data, 2000, 45, 457-460	2.8	17
1806	Liquid[liquid Equilibria of the System Water + 2-Propanol + 2,2,4-Trimethylpentane at 25 °C. Journal of Chemical & Data, 2000, 45, 898-901	2.8	17
1805	Water Activity in Polyol Systems. <i>Journal of Chemical & Chemical </i>	2.8	60
1804	Locating All Heterogeneous and Reactive Azeotropes in Multicomponent Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2000 , 39, 1576-1595	3.9	20
1803	Excess Enthalpies and Volumes of Ternary Mixtures Containing 1-Propanol or 1-Butanol, an Ether (Diisopropyl Ether or Dibutyl Ether), and Heptane. <i>Journal of Chemical & Discourage (Discourage (Disco</i>	2.8	38
1802	Conferring selectivity to chemical sensors via polymer side-chain selection: thermodynamics of vapor sorption by a set of polysiloxanes on thickness-shear mode resonators. 2000 , 72, 3696-708		70
1801	Experimental Results for the Limiting Activity Coefficients in Some Binary and Ternary Mixtures of Organic Components. <i>Journal of Chemical & Engineering Data</i> , 2000 , 45, 185-193	2.8	10
1800	Water Absorption by Secondary Organic Aerosol and Its Effect on Inorganic Aerosol Behavior. 2000 , 34, 71-77		100
1799	Group Definition in Molecular Solution Theories by Quantum Mechanical Methods: Application to 1-Alkanol +n-Alkane Mixtures. 2000 , 104, 11275-11282		22
1798	Engineering, Chemical Data Correlation. 2000 ,		
1797	Some chemical engineering applications of quantum chemical calculations. 2001 , 28, 313-351		2
1796	Densities, Viscosities, and Related Properties of Some (Methyl Ester + Alkane) Binary Mixtures in the Temperature Range from 283.15 to 313.15 K. <i>Journal of Chemical & Data</i> , 2001, 46, 974-983	2.8	59
1795	Linear free energy relationships used to evaluate equilibrium partitioning of organic compounds. 2001 , 35, 1-9		313
1794	Prediction of the acute toxicity (96-h LC50) of organic compounds to the fathead minnow (Pimephales promelas) using a group contribution method. 2001 , 14, 1378-85		124
1793	MODELLING OF PERVAPORATION: MODELS TO ANALYZE AND PREDICT THE MASS TRANSPORT IN PERVAPORATION. 2001 , 30, 49-125		97
1792	From UNIFAC to Modified UNIFAC (Dortmund) <i>Industrial & Industrial & I</i>	3.9	85
1791	Reactive Extraction. 2001,		40
	Thermodynamics of Ternary Mixtures Containing Sugars. SLE of d-Fructose in Pure and Mixed		

1789	Crystallization - Pages 536-575. 2001 , 536-575		1
1788	Thermodynamic modelling of aqueous aerosols containing electrolytes and dissolved organic compounds. 2001 , 32, 713-738		213
1787	Application of Group Contribution Models to the Calculation of the Octanol Water Partition Coefficient. <i>Industrial & Coefficient Coeffici</i>	3.9	16
1786	On the Hygroscopic Behavior of Atmospheric Organic Aerosols. <i>Industrial & Description of Atmospheric Organic Aerosols</i> .	3.9	31
1785	Prediction of Critical Micelle Concentrations of Nonionic Surfactants in Aqueous and Nonaqueous Solvents with UNIFAC. <i>Industrial & Engineering Chemistry Research</i> , 2001 , 40, 2362-2366	3.9	19
1784	LiquidIliquid Equilibria of the System Water + Acetic Acid + 2-Hexanone at 25 °C and 35 °C. <i>Journal of Chemical & Data</i> , 2001 , 46, 1452-1456	2.8	11
1783	Water Activity and pH in Aqueous Polycarboxylic Acid Systems. <i>Journal of Chemical & Engineering Data</i> , 2001 , 46, 582-587	2.8	29
1782	Azeotropes at Elevated Pressures for Systems Involving Cyclohexane, 2-Propanol, Ethyl Acetate, and Butanone. <i>Journal of Chemical & Engineering Data</i> , 2001 , 46, 1235-1238	2.8	8
1781	Predicting Cosolvency. 3. Evaluation of the Extended Log-Linear Model. <i>Industrial & Engineering Chemistry Research</i> , 2001 , 40, 5029-5035	3.9	11
1780	The CAPEC Database Journal of Chemical & Engineering Data, 2001, 46, 1041-1044	2.8	43
1779	Liquid Liquid Equilibria for the Ternary System Water + 2-Methyl-2-butanol + Diethylene Glycol Monobutyl Ether. <i>Journal of Chemical & Engineering Data</i> , 2001 , 46, 1530-1532	2.8	11
1778	Liquidliquid Equilibrium for tert-Amyl Ethyl Ether + Methanol + Water. <i>Journal of Chemical & Engineering Data</i> , 2001 , 46, 557-561	2.8	8
1777	Evaluation of the Group Contribution Activity Coefficient Models for the Calculation of the Thermodynamic Factor Relating to Self- and Mutual-Diffusion Coefficients in Polymer Solutions 2001 , 34, 1493-1498		3
1776	Modified UNIFAC (Dortmund). Reliable Model for the Development of Thermal Separation Processes 2001 , 34, 43-54		37
1775	Non-polar solutes in water and in aqueous solutions of protein denaturants. Modeling of solution and transfer processes. 2001 , 90, 183-202		14
1774	Prediction of water activity of osmotic solutions. 2001 , 49, 103-114		60
1773	Isothermal vaporlīquid equilibria for mixtures composed of 1,2-dimethoxybenzene, 2-methoxyphenol, and diphenylmethane. <i>Fluid Phase Equilibria</i> , 2001 , 178, 209-223	2.5	10
1772	Experimental and predicted excess molar volumes and excess molar enthalpies for di-n-butyl ether + 1-propanol + n-octane at 298.15 and 308.15 K. <i>Fluid Phase Equilibria</i> , 2001 , 179, 363-383	2.5	7

(2001-2001)

1771	FT-IR spectroscopic investigations of hydrogen bonding in alcoholflydrocarbon solutions. <i>Fluid Phase Equilibria</i> , 2001 , 186, 1-25	2.5	119	
1770	The application of the equations of state incorporated with mixing rules for viscosity estimations of binary mixtures. <i>Fluid Phase Equilibria</i> , 2001 , 181, 47-58	2.5	32	
1769	Analysis of infinite dilution activity coefficients of solutes in hydrocarbons from UNIFAC. <i>Fluid Phase Equilibria</i> , 2001 , 181, 163-186	2.5	20	
1768	Volumetric properties and viscosities of the methyl butanoate + n-heptane + n-octane ternary system and its binary constituents in the temperature range from 283.15 to 313.15 K. <i>Fluid Phase Equilibria</i> , 2001 , 186, 207-234	2.5	74	
1767	Liquid[Iquid equilibria of ternary 2M1B/2M2BIM1BOH日2O and quaternary 2M1BIM2BIM1BOH日2O mixtures. <i>Fluid Phase Equilibria</i> , 2001 , 187-188, 415-424	2.5	5	
1766	Boiling points for five binary systems of sulfolane with aromatic hydrocarbons at 101.33 kPa. <i>Fluid Phase Equilibria</i> , 2001 , 190, 61-71	2.5	14	
1765	Solubility of the tralol in pure carbon dioxide and in a mixed solvent formed by ethanol and carbon dioxide. <i>Fluid Phase Equilibria</i> , 2001 , 191, 59-69	2.5	6	
1764	A modified PSRK model for the prediction of the vaporliquid equilibria of asymmetric systems. <i>Fluid Phase Equilibria</i> , 2001 , 192, 103-120	2.5	9	
1763	Excess enthalpies of alkanediamines+benzene or + toluene mixtures. 2001 , 369, 1-7		5	
1762	Combining solvent engineering and thermodynamic modeling to enhance selectivity during monoglyceride synthesis by lipase-catalyzed esterification. 2001 , 28, 362-369		75	
1761	Equilibrium constant for lipase-catalyzed condensation of mannose and lauric acid in water-miscible organic solvents. 2001 , 29, 494-498		25	
1760	New process for separating propylene and propane by extractive distillation with aqueous acetonitrile. 2001 , 84, 581-586		36	
1759	(Liquid + liquid) equilibria of (tert -amyl ethyl ether+ ethanol + water) at several temperatures. 2001 , 33, 139-146		14	
1758	A method of estimating multicomponent nonaqueous-phase liquid mass in porous media using aqueous concentration ratios. 2001 , 20, 2443-2449		2	
1757	Optimization of carbohydrate fatty acid ester synthesis in organic media by a lipase from Candida antarctica. 2001 , 74, 483-91		122	
1756	Liquid-liquid extraction of aroma compounds with hollow fiber contactor. AICHE Journal, 2001, 47, 1780	- <u>3</u> .893	77	
1755	Primary nucleation of paracetamol in acetoneWater mixtures. 2001 , 56, 2305-2313		84	
1754	Separation of chlorobenzoic acids by dissociation extractive crystallization. 2001 , 56, 2335-2346		3	

1753	The hygroscopic properties of dicarboxylic and multifunctional acids: measurements and UNIFAC predictions. 2001 , 35, 4495-501	418
1752	Prediction of Infinite Dilution Volatilities of Aroma Compounds in Water. 2001 , 66, 447-452	9
1751	The effect of water on gasparticle partitioning of secondary organic aerosol. Part I: pinene/ozone system. 2001 , 35, 6049-6072	169
1750	Calorimetric Behaviour of Primary Bromobutanes with Isomeric Butanols. 2001 , 215,	11
1749	Experimental Investigations of Oxygenated Gasoline Dissolution. 2001 , 127, 208-216	21
1748	A new Monte Carlo simulation approach for the prediction of sorption equilibria of oligomers in polymer melts: Solubility of long alkanes in linear polyethylene. 2001 , 115, 2860-2875	29
1747	Hygroscopic Study of Glucose, Citric Acid, and Sorbitol Using an Electrodynamic Balance: Comparison with UNIFAC Predictions. 2001 , 35, 753-758	58
1746	Simultaneous Synthesis and Design of Novel Chemicals and Chemical Process Flowsheets. 2002 , 10, 115-120	5
1745	Flake Drying Temperature Affects Mat Properties during Pressing. 2002, 56, 558-562	7
1744	Solvent Effects on Equilibrium Position and Initial Rate of Lipase-catalyzed Esterification Reactions in Organic Solvents: Experimental Results and Prediction Capabilities. 2002 , 20, 101-109	9
1743	Predicting adhesion between a crystalline polymer and silane-treated glass surfaces in filled composites. 2002 , 16, 1949-1956	10
1742	The prediction of adhesion between polymer matrices and silane-treated glass surfaces in filled composites. 2002 , 16, 495-507	9
1741	Liquid-Liquid equilibria of the water-acetic acid-butyl acetate system. 2002 , 19, 243-254	39
1740	Computer-Aided Chemical Engineering. 2002,	
1739	Liquid Liquid Liquid Equilibrium of Diisopropyl Ether + Ethanol + Water System at Different Temperatures. <i>Journal of Chemical & Data</i> , 2002, 47, 529-532	25
1738	UNIFAC-FV Applied to Dendritic Macromolecules in Solution: Comment on Vapor Liquid Equilibria for Dendritic-Polymer Solutions (Lieu, J. G.; Liu, M.; Fr Libhet, J. M. J.; Prausnitz, J. M. J. Chem. Eng. 2.8 Data 1999, 44, 613 § 200). Journal of Chemical & Engineering Data, 2002, 47, 376-377	5
1737	Isobaric Vapor Liquid Equilibria of Diethyl Carbonate with Four Alkanes at 101.3 kPa. <i>Journal of Chemical & Data</i> , 2002 , 47, 1098-1102	33
1736	Liquid Liquid Equilibria for the Ternary System Water + Octane + Diethylene Glycol Monobutyl Ether. Journal of Chemical & amp; Engineering Data, 2002, 47, 310-312	22

1735	Density-modified displacement for dense nonaqueous-phase liquid source-zone remediation: density conversion using a partitioning alcohol. 2002 , 36, 2082-7		37
1734	Free-Volume Activity Coefficient Models for Dendrimer Solutions. <i>Industrial & Description of the Models for Dendrimer Solutions</i> . <i>Industrial & Description of the Models for Dendrimer Solutions</i> . <i>Industrial & Description of the Models for Dendrimer Solutions</i> . <i>Industrial & Description of the Models for Dendrimer Solutions</i> . <i>Industrial & Description of the Models for Dendrimer Solutions</i> . <i>Industrial & Dendrimer Solutions</i> .	3.9	15
1733	Total Vapor Pressure Measurements for 2-Ethoxyethanol with Methanol, Ethanol, 1-Propanol, and 2-Propanol at 313.15 K. <i>Journal of Chemical & Engineering Data</i> , 2002 , 47, 1355-1358	2.8	12
1732	A Comment on Guggenheim-like Hard-Core Volume Expressions. <i>Industrial & Description of Chemistry Research</i> , 2002 , 41, 4686-4688	3.9	2
1731	Liquid Liquid and Solid Liquid Equilibria in Systems Containing n-Eicosane, n-Tetracosane, Ethanol, and Water. <i>Journal of Chemical & amp; Engineering Data</i> , 2002 , 47, 106-109	2.8	3
1730	Vaporliquid Equilibrium for Propionic Acid + n-Butyl Propionate from 60 to 101.3 kPa. <i>Journal of Chemical & Engineering Data</i> , 2002 , 47, 1367-1371	2.8	7
1729	Interfacial tension of chlorinated aliphatic DNAPL mixtures as a function of organic phase composition. 2002 , 36, 1292-8		14
1728	Thermophysical Properties of Acetone or Methanol + n-Alkane (C9 to C12) Mixtures. <i>Journal of Chemical & Company Engineering Data</i> , 2002 , 47, 887-893	2.8	50
1727	Implications of alcohol partitioning behavior for in situ density modification of entrapped dense nonaqueous phase liquids. 2002 , 36, 104-11		22
1726	Extension of the ElliottBureshDonohue Equation of State to Polymer Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 1043-1050	3.9	16
1725	Kinematic Viscosities of Poly(ethylene glycol) Blends. <i>Journal of Chemical & Data</i> , 2002 , 47, 835-838	2.8	3
1724	Development of a Universal Group Contribution Equation of State. 2. Prediction of Vaporliquid Equilibria for Asymmetric Systems. <i>Industrial & Equilibria Chemistry Research</i> , 2002 , 41, 3489-3498	₃ 3.9	92
1723	Development of a Universal Group Contribution Equation of State III. Prediction of Vapor liquid Equilibria, Excess Enthalpies, and Activity Coefficients at Infinite Dilution with the VTPR Model. <i>Industrial & Dilution amp; Engineering Chemistry Research</i> , 2002 , 41, 5890-5899	3.9	66
1722	Thermodynamic Modeling and Process Optimization of Supercritical Fluid Fractionation of Fish Oil Fatty Acid Ethyl Esters. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 1516-1527	3.9	50
1721	UNIFAC Parameters for Four New Groups. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 2047-2057	3.9	32
1720	Kinetics of Catalytic Esterification of Propionic Acid and n-Butanol over Amberlyst 35. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 2882-2887	3.9	68
1719	A Priori Phase Equilibrium Prediction from a Segment Contribution Solvation Model. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 899-913	3.9	564
1718	A Modified UNIFAC (Dortmund) Model. 4. Revision and Extension. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 1678-1688	3.9	160

1717	The estimation of melting points and fusion enthalpies using experimental solubilities, estimated total phase change entropies, and mobile order and disorder theory. 2002 , 42, 368-74		20
1716	Semi-empirical strategies for predicting adhesion. 2002 , 1-73		4
1715	New Hybrid Neural Network Model for Prediction of Phase Equilibrium in a Two-Phase Extraction System. <i>Industrial & Description of Phase Equilibrium in a Two-Phase Extraction 3.9</i>	ı	5
1714	Prediction of physico-chemical properties for PCs/DFs using the UNIFAC model with an alternative approximation for group assignment. 2002 , 49, 135-42		8
1713	Nonlinear Structure Affinity Relationships for Vapor Guest Inclusion by Solid Calixarenes. 2002 , 106, 5845-5851		45
1712	Manipulation of the Liquid Liquid Equilibrium of Vertrel-XF + Hydrocarbon Solvent Systems with the Addition of a Third Component. <i>Industrial & Engineering Chemistry Research</i> , 2002 , 41, 2792-279 ³⁻⁹		7
1711	Modeling of gas solubility in brine. 2002 , 33, 635-642		39
1710	Studies on the Extraction of Aromatics from C9+ Oil 2002 , 35, 1257-1262		7
1709	Thermodynamic modelling of phase equilibrium for water + poly(Ethylene glycol) + salt aqueous two-phase systems. 2002 , 19, 255-266		25
1708	Mixture Evaporative Characteristics Prediction for LIF Measurements Using PSRK (Predictive Soave-Redlich-Kwong) Equation of State. 2002 ,		10
1707	Size as a parameter for solvent effects on Candida antarctica lipase B enantioselectivity. 2002 , 1594, 325-34		69
1706	Applied thermodynamics for process modeling. <i>AICHE Journal</i> , 2002 , 48, 194-200 3.6		125
1705	Fast solvent screening via quantum chemistry: COSMO-RS approach. <i>AICHE Journal</i> , 2002 , 48, 369-385 3.6		1127
1704	Screening of cosolvents for a supercritical fluid: A fully predictive approach. <i>AICHE Journal</i> , 2002 , 48, 551-560		8
1703	Thermodynamic equilibrium of organic-electrolyte mixtures in aerosol particles. <i>AICHE Journal</i> , 2002 , 48, 1331-1348		94
1702	COSMOSPACE: Alternative to conventional activity-coefficient models. <i>AICHE Journal</i> , 2002 , 48, 2332-2348		114
1701	Phase equilibrium engineering of supercritical hydrogenation reactors. <i>AICHE Journal</i> , 2002 , 48, 2635-26 4.5		28
1700	Calculation of solubilities of the pesticides diuron and monuron in organic nonelectrolyte solvents using UNIFAC and modified UNIFAC (dortmund) models. 2002 , 80, 530-535		

1699	An extension of the group contribution model for thermodynamic and transport properties of dilute gases. 2002 , 19, 843-862		7
1698	Comparison of methods for extraction, storage, and silylation of pentafluorobenzyl derivatives of carbonyl compounds and multi-functional carbonyl compounds. 2002 , 372, 808-16		20
1697	Phase equilibria in mixtures of fatty oils and derivatives with near critical fluids using the GC-EOS model. 2002 , 23, 91-102		107
1696	Universal method for equations of state (UNIFEST): An application of UNIFAC to predict the parameters of cubic equations of state. <i>Fluid Phase Equilibria</i> , 2002 , 193, 75-86	2.5	4
1695	Evaluation of equations of state applicable to polymers and complex systems. <i>Fluid Phase Equilibria</i> , 2002 , 194-197, 77-86	2.5	25
1694	Thermodynamic modeling of biomass conversion processes. Fluid Phase Equilibria, 2002, 194-197, 805-8	3 125 5	24
1693	Isobaric vapourllquid equilibria of dimethyl carbonate with alkanes and cyclohexane at 101.3 kPa. <i>Fluid Phase Equilibria</i> , 2002 , 198, 95-109	2.5	41
1692	Solubilities of terephthalaldehydic, p-toluic, benzoic, terephthalic and isophthalic acids in N,N-dimethylformamide from 294.75 to 370.45 K. <i>Fluid Phase Equilibria</i> , 2002 , 200, 69-74	2.5	68
1691	LiquidIIquid equilibria of a hydrofluoroether + water + ethanol system. <i>Fluid Phase Equilibria</i> , 2002 , 201, 97-106	2.5	
1690	Revision of UNIFAC group interaction parameters of group contribution models to improve prediction results of vaporliquid equilibria for solventpolymer systems. <i>Fluid Phase Equilibria</i> , 2002 , 202, 367-383	2.5	10
1689	Development of GEQUAC as a new group contribution method for strongly non-ideal mixtures. <i>Fluid Phase Equilibria</i> , 2002 , 203, 53-69	2.5	10
1688	Vapourliquid equilibria of dimethyl carbonate with linear alcohols and estimation of interaction parameters for the UNIFAC and ASOG method. <i>Fluid Phase Equilibria</i> , 2002 , 201, 187-201	2.5	59
1687	Performance simulation of an absorption heat transformer operating with partially miscible mixtures. 2002 , 72, 583-597		9
1686	Phase equilibrium and diffusion of solvents in polybutadiene: A capillary-column inverse gas chromatography study. 2002 , 40, 1046-1055		9
1685	Used Motor Oil as a Source of MTBE, TAME, and BTEX to Ground Water. 2002, 22, 46-51		12
1684	Water activities of florinated solid polymer electrolyte/water systems using group-contribution method. 2002 , 57, 2747-2752		3
1683	Global optimization for clusters of flexible moleculesBolventBolute interaction energy calculations. <i>Fluid Phase Equilibria</i> , 2002 , 194-197, 169-183	2.5	10
1682	Liquid II quid equilibria of limonene+linalool+diethylene glycol system at different temperatures. 2002 , 89, 223-227		24

1681	Analog calorimetry and UNIQUAC group contributions approaches to the miscibility of pvc with eva copolymers. 2002 , 70, 927-947		5
1680	Sugar monomer and oligomer solubility: data and predictions for application to biomass hydrolysis. 2003 , 105 -108, 179-93		53
1679	Blend formation between homo- and co-polymers at 298.15 k, PMMA-SAN blends. 2003, 71, 353-365		3
1678	The effect of multicomponent diffusion on NAPL dissolution from spherical ternary mixtures. 2003 , 67, 43-60		7
1677	Heterogeneous batch-extractive distillation of minimum boiling azeotropic mixtures. <i>AICHE Journal</i> , 2003 , 49, 3074-3083	3.6	37
1676	Optimal solvent design for batch separation based on economic performance. <i>AICHE Journal</i> , 2003 , 49, 3095-3109	3.6	63
1675	Thermodynamic parameters monitoring the equilibrium shift of enzyme-catalyzed hydrolysis/synthesis reactions in favor of synthesis in mixtures of water and organic solvent. 2003 , 81, 167-77		11
1674	Solid-phase peptide synthesis by ion-paired alpha-chymotrypsin in nonaqueous media. 2003 , 81, 809-17		27
1673	Unexpected behavior between polystyrene and untreated and silane-treated glass beads in filled polymeric composites. 2003 , 89, 521-526		2
1672	A new model for predicting activity coefficients in aqueous solutions of amino acids and peptides. 2003 , 35, 101-112		27
1671	The QCHB model of fluids and their mixtures. 2003 , 35, 349-381		39
1670	(Liquid + liquid) equilibria of (water + ethanol + dimethyl glutarate) at several temperatures. 2003 , 35, 1671-1679		28
1669	Analysis and critical comparison of the reversed-phase and ion-exchange contributions to retention on polybutadiene coated zirconia and octadecyl silane bonded silica phases. 2003 , 996, 13-31		98
1668	Comparison of various models for transport of binary mixtures through dense polymer membrane. 2003 , 44, 2679-2687		35
1667	Application of IR-spectroscopy in thermodynamic investigations of associating solutions. <i>Fluid Phase Equilibria</i> , 2003 , 205, 195-214	2.5	21
1666	Surface and interfacial tensions of the systems water + n-butyl acetate + methanol and water + n-pentyl acetate + methanol at 303.15 K. <i>Fluid Phase Equilibria</i> , 2003 , 208, 1-21	2.5	59
1665	Solvent activities of ordinary and associated binary polymer solutions: group-contribution method. <i>Fluid Phase Equilibria</i> , 2003 , 207, 247-261	2.5	3
1664	Simultaneous description of excess properties and vaporliquid equilibria for associating mixtures by hydrogen-bonding lattice fluid equation of state. <i>Fluid Phase Equilibria</i> , 2003 , 212, 221-231	2.5	5

1663	The sizes of moleculesEevisited. 2003 , 16, 398-408		32
1662	Estimation of equilibrium properties in formulation or processing of liquid foods. 2003 , 82, 41-49		9
1661	Solid[]quid and liquid[]quid equilibria for 1,3,5-trioxane, or 1,4,7,10,13,16-hexaoxacyclooctadecane + selected n-alkane mixtures: Analysis in terms of DISQUAC. <i>Fluid Phase Equilibria</i> , 2003 , 205, 317-338	2.5	17
1660	Propanediols for separation of citrus oil: liquid[]quid equilibria of limonene + linalool + (1,2-propanediol or 1,3-propanediol). <i>Fluid Phase Equilibria</i> , 2003 , 211, 129-140	2.5	29
1659	Quantum mechanics: a new tool for engineering thermodynamics. Fluid Phase Equilibria, 2003, 210, 147-	160	17
1658	Predicting aqueous solubilities from aqueous free energies of solvation and experimental or calculated vapor pressures of pure substances. 2003 , 119, 1661-1670		88
1657	Lipase-catalyzed synthesis of xylitol monoesters: solvent engineering approach. 2003, 102, 251-9		97
1656	Isobaric Phase Equilibria of Diethyl Carbonate with Five Alcohols at 101.3 kPa. <i>Journal of Chemical & Engineering Data</i> , 2003 , 48, 86-91	2.8	38
1655	Equation-of-State Models and Quantum Mechanics Calculations. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 1495-1507	3.9	28
1654	A New Phase-Equilibrium Model for Simulating Industrial Nylon-6 Production Trains. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 3900-3913	3.9	24
1653	Vaporliquid Equilibrium and Volumetric Measurements for Binary Mixtures of 1,4-Dioxane with Isomeric Chlorobutanes. <i>Journal of Chemical & Engineering Data</i> , 2003 , 48, 887-891	2.8	20
1652	Liquidliquid Equilibria for the Epichlorohydrin + Water + Methanol and Allyl Chloride + Water + Methanol Systems. <i>Journal of Chemical & Data</i> , 2003, 48, 1015-1018	2.8	8
1651	Predicting Vaporization of Residua by UNIFAC Model and Its Implications to RFCC Operations. 2003 , 17, 631-636		10
1650	A Parametric Study of Dipolar Chain Theory with Applications to Ketone Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 5687-5696	3.9	54
1649	Aerosol organic-mass-to-organic-carbon ratio measurements. 2003 , 37, 2982-7		192
1648	Experimental and Theoretical Analysis of Phase Equilibria in a Two-phase System Used for Biocatalytic Esterifications. 2003 , 21, 115-121		13
1647	Vaporliquid Equilibria by UNIFAC Group Contribution. 6. Revision and Extension. <i>Industrial & Engineering Chemistry Research</i> , 2003 , 42, 183-188	3.9	224
1646	Thermodynamic modelling of aqueous aerosols containing electrolytes and dissolved organic compounds. II. An extended ZdanovskiiBtokesRobinson approach. 2003 , 34, 667-690		101

1645	Effect of silane coupling agent adsorbate structure on adhesion performance with a polymeric matrix. 2003 , 34, 327-332	49
1644	Thermodynamics of mixtures containing a very strongly polar compound: IV lapplication of the DISQUAC, UNIFAC and ERAS models to DMSO+ organic solvent systems. 2003 , 41, 583-597	17
1643	Prediction of Infinite Dilution Activity Coefficients Using COSMO-RS. <i>Industrial & Dilution Activity Research</i> , 2003 , 42, 3635-3641	74
1642	Measurement and Prediction of Quaternary Azeotropes for Cyclohexane + 2-Propanol + Ethyl Acetate + Butanone System at Elevated Pressures. <i>Journal of Chemical & Data</i> , 2.8 2003 , 48, 66-70	4
1641	Predicting the Solubilities of Complex Chemicals I. Solutes in Different Solvents. <i>Industrial & amp; Engineering Chemistry Research</i> , 2003 , 42, 5622-5634	45
1640	Chapter 6 Phase equilibria. 2003 , 13, 181-226	
1639	Emission and fate assessment of methyl tertiary butyl ether in the Boston area airshed using a simple multimedia box model: comparison with urban air measurements. 2003 , 53, 1426-35	6
1638	Sugar Monomer and Oligomer Solubility. 2003 , 179-193	7
1637	Property Calculation and Prediction for Selecting Solvent Systems in CCC. 2003, 26, 1397-1415	15
1636	Volatile Fuel Hydrocarbons and MTBE in the Environment. 2003 , 433-474	8
1635	MODELLING THE HYGROSCOPIC PROPERTIES OF AEROSOLS. 2004 , 35, S961-S962	
1634	. 2004,	2
1633	Volatilization of Binary Nonaqueous Phase Liquid Mixtures in Unsaturated Porous Media. 2004 , 3, 645-655	12
1632	Modelling Phase Equilibria in Systems with Organic Solid Solutions. 2004 , 229-249	4
1631	Limiting activity coefficients of aqueous flavour systems at 298 K by the group contribution solvation (GCS) model. 2004 , 102, 235-241	5
1630	Models for Liquid Phase Activity Coefficients - UNIFAC. 2004 , 19, 59-74	3
1629	HCToolkit/EOS interface: an open source, multi-platform phase equilibria framework for exploring phase behaviour of complex mixtures. 2004 , 237, 89-98	1
1628	Challenges in thermodynamics. 2004 , 43, 221-238	34

1627	Reaction equilibrium for lipase-catalyzed condensation in organic solvent systems. 2004 , 26, 1461-8		19
1626	Design Directions for Composite Catalytic Hollow Fibre Membranes for Condensation Reactions. 2004 , 82, 220-228		24
1625	LiquidIiquid Equilibria of Linalool + Ethanol + Water, Water + Ethanol + Limonene, and Limonene + Linalool + Water Systems. 2004 , 33, 561-569		35
1624	Methods to assess the amenability of petroleum hydrocarbons to bioremediation. 2004 , 23, 929-37		9
1623	Water solubility and partitioning behavior of brominated phenols. 2004 , 23, 1386-93		45
1622	Predicting infinite dilution activity coefficients with the group contribution solvation model: an extension of its applicability to aqueous systems. <i>Fluid Phase Equilibria</i> , 2004 , 221, 127-137	2.5	10
1621	VLE predictions with the PengRobinson equation of state and temperature dependent kij calculated through a group contribution method. <i>Fluid Phase Equilibria</i> , 2004 , 224, 285-304	2.5	289
1620	Measurements of sorption isotherms and diffusion coefficients by means of a magnetic suspension balance. 2004 , 43, 753-763		50
1619	Acrylic acid/vinyl acetate suspension copolymerizations. I. Partition coefficients for acrylic acid. 2004 , 93, 1077-1088		9
1618	Thermodynamics of fluid-phase equilibria for standard chemical engineering operations. <i>AICHE Journal</i> , 2004 , 50, 739-761	3.6	155
1617	Air pollution: A half century of progress. AICHE Journal, 2004, 50, 1096-1108	3.6	67
1616	Estimation of infinite dilution activity coefficients of organic compounds in water with neural classifiers. <i>AICHE Journal</i> , 2004 , 50, 1315-1343	3.6	20
1615	Solubility, dissolution rate and phase transition studies of ranitidine hydrochloride tautomeric forms. 2004 , 282, 73-85		54
1614	Correlation of activity coefficients of alkyl-ammonium salt solutions. 2004 , 113, 21-27		1
1613	Experimental solid + liquid equilibria and excess molar volumes of alkanol + hexylamine mixtures. <i>Fluid Phase Equilibria</i> , 2004 , 216, 135-145	2.5	24
1612	Vapor-phase chemical equilibrium for the hydrogenation of benzene to cyclohexane from reaction-ensemble molecular simulation. <i>Fluid Phase Equilibria</i> , 2004 , 219, 181-193	2.5	16
1611	Vaporllquid equilibria in dendrimer and hyperbranched polymer solutions: experimental data and modeling using UNIFAC-FV. <i>Fluid Phase Equilibria</i> , 2004 , 221, 83-96	2.5	18
1610	Phase stability of the system limonene+linalool+2-aminoethanol. <i>Fluid Phase Equilibria</i> , 2004 , 226, 121-	1 2 .75	18

1609	Liquid I quid equilibria for mixtures of {methyl acetate + methanol + n-alkane (C10 I 12)} at several temperatures and 1 atm. 2004 , 36, 237-243		7
1608	A free-volume modification of GEM-QC to correlate VLE and LLE in polymer solutions. 2004 , 36, 409-41	7	9
1607	(Liquid+liquid) equilibria for (water+acetic acid+2-ethyl-1-hexanol): experimental data and prediction. 2004 , 36, 1001-1006		39
1606	LiquidIquid equilibria for butyl tert-butyl ether + (methanol or ethanol) + water at several temperatures. <i>Fluid Phase Equilibria</i> , 2004 , 224, 185-192	2.5	23
1605	Group contribution method with SAFT EOS applied to vapor liquid equilibria of various hydrocarbon series. <i>Fluid Phase Equilibria</i> , 2004 , 222-223, 67-76	2.5	142
1604	Vapourliquid equilibrium and azeotropic behaviour of 1,2-dichloroethane with isomeric butanols. <i>Fluid Phase Equilibria</i> , 2004 , 225, 77-83	2.5	8
1603	Densities and Excess Molar Properties of Dimethyl Carbonate with Alkanes (C6to C10) and VLE of Dimethyl Carbonate with Alkanes (C9to C10) at 101.3 kPa. <i>Journal of Chemical & Data</i> , 2004, 49, 86-93	2.8	28
1602	DISQUAC Predictions on Thermodynamic Properties of Ternary and Higher Multicomponent Mixtures. 3. Results forHEof Ternary Mixtures Containing One Alcohol, One Polar Compound, and One Hydrocarbon or a Polar Compound, or Three Alkanols.	3.9	15
1601	Deliquescence and Crystallization of Ammonium Sulfate Particles Internally Mixed with Water-Soluble Organic Compounds. 2004 , 108, 11600-11608		101
1600	Experimental and Predicted Solubilities of HFC134a (1,1,1,2-Tetrafluoroethane) in Polyethers. <i>Industrial & Discourse amp; Engineering Chemistry Research</i> , 2004 , 43, 1523-1529	3.9	17
1599	Comparison of an empirical and a theoretical linear solvation energy relationship applied to the characterization of solute distribution in a poly(ethylene) glycol-salt aqueous biphasic system. 2004 , 44, 549-58		5
1598	Improvement of the ZdanovskiiBtokesRobinson Model for Mixtures Containing Solutes of Different Charge Types. 2004 , 108, 1008-1017		84
1597	Experimental Solid + Liquid Equilibria and Excess Molar Volume of Alkanol + Octylamine Mixtures. Analysis in Terms of ERAS, DISQUAC, and Modified UNIFACII <i>Journal of Chemical & Data</i> , 2004 , 49, 101-108	2.8	21
1596	Acoustically enhanced multicomponent NAPL ganglia dissolution in water saturated packed columns. 2004 , 38, 2940-5		14
1595	Liquid Liquid Equilibria of Methyl Acetate + Methanol + Octane or Nonane. <i>Journal of Chemical & Engineering Data</i> , 2004 , 49, 664-667	2.8	3
1594	Volumetric and Solid + Liquid Equilibrium Data for Linear 1-Alkanol + Decylamine Mixtures. Analysis in Terms of ERAS, DISQUAC, and Modified UNIFACII <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 7647-7656	3.9	18
1593	Deliquescence of malonic, succinic, glutaric, and adipic acid particles. 2004 , 109, n/a-n/a		76
1592	Solubility Modeling with a Nonrandom Two-Liquid Segment Activity Coefficient Model. <i>Industrial & Engineering Chemistry Research</i> , 2004 , 43, 8354-8362	3.9	165

1591	Nonrandom Hydrogen-Bonding Model of Fluids and Their Mixtures. 1. Pure Fluids. <i>Industrial & amp;</i> Engineering Chemistry Research, 2004 , 43, 6592-6606 3.9	91
1590	Prediction of Thermodynamic Properties of the Systems Formed by n-Alkanes, Aliphatic Monoethers, and 1-Chloroalkanes, Using a CellHole Group Contribution Model. 2004 , 108, 2383-2397	7
1589	Partition Coefficients of Organic Solutes between Supercritical Carbon Dioxide and Water: Experimental Measurements and Empirical Correlations. <i>Journal of Chemical & Empirical Correlations</i> 2.8 Data, 2004 , 49, 768-778	29
1588	The European Bioinformatics Institute Macromolecular Structure Relational Database Technology. 223-240	2
1587	Liquid-liquid equilibria of propionic acid - water - solvent (n-hexane, cyclohexane, cyclohexanol and cyclohexyl acetate) ternaries at 298.15 K. 2004 , 21, 647-657	30
1586	Volatilization of Binary Nonaqueous Phase Liquid Mixtures in Unsaturated Porous Media. 2004 , 3, 645-655	1
1585	Water activity in polyol/water systems: new UNIFAC parameterization. 2005, 5, 1545-1555	72
1584	Application of several activity coefficient models to water-organic-electrolyte aerosols of atmospheric interest. 2005 , 5, 2475-2495	67
1583	Reactive Extraction: Principles and Apparatus Concepts. 2005, 313-337	1
1582	Effect of water activity on gibberellic acid production by Gibberella fujikuroi under solid-state fermentation conditions. 2005 , 40, 2655-2658	29
1581	Extension of the Wilson model to multicomponent polymer solutions: applications to polymer polymer aqueous two-phase systems. 2005 , 37, 55-60	35
1580	(Liquid+liquid) equilibria of (water+butyric acid+cyclohexyl acetate) ternary system. 2005 , 37, 175-180	32
1579	VLE of the binary systems (dimethyl carbonate with 2-propanol or 2-butanol) and (diethyl carbonate with methylcyclohexane) at 101.3 kPa. 2005 , 37, 249-257	17
1578	(Liquid+liquid) equilibria of (water+butyric acid+isoamyl alcohol) ternary system. 2005 , 37, 297-303	34
1577	(Liquid+liquid) equilibria of (water+propionic acid+dimethyl phthalate) at several temperatures. 2005 , 37, 837-842	34
1576	(Liquid+liquid) equilibrium of (dibutyl ether+methanol+water) at different temperatures. 2005 , 37, 1007-101	2 8
1575	(Liquid + liquid) equilibria of (water + propionic acid + diethyl phthalate) at several temperatures. 2005 , 37, 1144-1150	24
1574	(Liquid+liquid) equilibria of (water+propionic acid+cyclohexanone) at several temperatures. 2005 , 37, 1288-1293	31

1573	Systems with ionic liquids: Measurement of VLE and Plata and prediction of their thermodynamic behavior using original UNIFAC, mod. UNIFAC(Do) and COSMO-RS(Ol). 2005 , 37, 603-619		368
1572	A predictive thermodynamic model for the Brazilian gasoline. 2005 , 84, 1099-1104		19
1571	A study of packing induced selectivity effects in the liquid phase adsorption of alkane/alkene mixtures on NaY. 2005 , 82, 191-199		24
1570	Supramolecular structure and physicochemical properties of the trichloromethanethenol mixtures. 2005 , 121, 127-138		10
1569	Vaporliquid equilibria in the binary system (⊪beta-pinene+(+)-fenchone. Fluid Phase Equilibria, 2005 , 227, 113-124	2.5	4
1568	Extension of the A-UNIFAC model to mixtures of cross- and self-associating compounds. <i>Fluid Phase Equilibria</i> , 2005 , 227, 165-176	2.5	32
1567	LiquidIquid equilibria of the ternary system water+acetic acid+dimethyl adipate. <i>Fluid Phase Equilibria</i> , 2005 , 230, 58-63	2.5	39
1566	Prediction and experimental verification of the effect of salt on the vapourlquid equilibrium of ethanol/1-propanol/water mixture. <i>Fluid Phase Equilibria</i> , 2005 , 234, 84-93	2.5	12
1565	Octanol-water partition coefficient of glucose, sucrose, and trehalose. 2005 , 340, 1207-11		48
1564	Pure component properties from group contribution: Hydrogen-bond basicity, hydrogen-bond acidity, Hildebrand solubility parameter, macroscopic surface tension, dipole moment, refractive index and dielectric constant. <i>Fluid Phase Equilibria</i> , 2005 , 231, 27-37	2.5	34
1563	Extension of the NRTL and NRF models to multicomponent polymer solutions: Applications to polymer polymer aqueous two-phase systems. <i>Fluid Phase Equilibria</i> , 2005 , 231, 77-83	2.5	26
1562	Extension of the group contribution associating equation of state to mixtures containing phenol, aromatic acid and aromatic ether compounds. <i>Fluid Phase Equilibria</i> , 2005 , 231, 197-210	2.5	18
1561	Vapourliquid equilibrium for the 2-methylpropane+methanol, +ethanol, +2-propanol, +2-butanol and +2-methyl-2-propanol systems at 313.15K. <i>Fluid Phase Equilibria</i> , 2005 , 232, 90-99	2.5	16
1560	Extension of linear isotherm regularity to long chain primary, secondary and tertiary alcohols, ketones and 1-carboxylic acids by group contribution method. <i>Fluid Phase Equilibria</i> , 2005 , 234, 11-21	2.5	14
1559	Volume, surface and UNIQUAC interaction parameters for imidazolium based ionic liquids via Polarizable Continuum Model. <i>Fluid Phase Equilibria</i> , 2005 , 234, 64-76	2.5	176
1558	Vapor I lquid equilibria for the quaternary reactive system ethyl acetate + ethanol + water + acetic acid and some of the constituent binary systems at 101.3 kPa. <i>Fluid Phase Equilibria</i> , 2005 , 235, 215-222	2.5	51
1557	Experimental and predicted vapourliquid equilibrium of 1,4-dioxane with cycloalkanes and benzene. <i>Fluid Phase Equilibria</i> , 2005 , 238, 1-6	2.5	10
1556	Liquid I quid equilibria of the ternary system water+acetic acid+dimethyl succinate. Fluid Phase Equilibria, 2005, 238, 33-38	2.5	14

1555	Performance of a Conductor-Like Screening Model for Real Solvents Model in Comparison to Classical Group Contribution Methods. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 1610-1624	131
1554	An improved prediction result of entropic-FV model for vaporllquid equilibria of solventpolymer systems. 2005 , 97, 1145-1153	6
1553	Modeling high-pressure wax formation in petroleum fluids. <i>AICHE Journal</i> , 2005 , 51, 2089-2097 3.6	20
1552	Crystal growth rates of paracetamol in mixtures of water + acetone + toluene. <i>AICHE Journal</i> , 2005 , 51, 2441-2456	20
1551	A free-volume term based on the van der Waals partition function for the UNIFAC model. <i>Fluid Phase Equilibria</i> , 2005 , 228-229, 321-328	33
1550	Applied thermodynamics in chemical technology: current practice and future challenges. <i>Fluid Phase Equilibria</i> , 2005 , 228-229, 49-57	14
1549	Thermodynamics of mixtures with strongly negative deviations from Raoult's law: Part 9. Vaporllquid equilibria for the system 1-propanol + di-n-propylamine at six temperatures between 2.5 293.15 and 318.15 K. <i>Fluid Phase Equilibria</i> , 2005 , 231, 211-220	25
1548	A modified free-volume-based model for predicting vaporliquid and solidliquid equilibria for size asymmetric systems. <i>Fluid Phase Equilibria</i> , 2005 , 234, 94-100	16
1547	Vaporllquid equilibria for systems of diethyl carbonate and ketones and determination of group interaction parameters for the UNIFAC and ASOG methods. <i>Fluid Phase Equilibria</i> , 2005 , 235, 83-91	11
1546	Application of UNIFACIIdWBV model to waterBEO systems. Fluid Phase Equilibria, 2005, 237, 86-88 2.5	5
1545	New expressions for non-randomness in equation-of-state models. Fluid Phase Equilibria, 2005, 237, 130-1399	12
1544	(Liquid+liquid) equilibria of the (water+acetic acid+dibutyl phthalate) system. 2005 , 37, 1256-1260	13
1543	A modified entropic expression for the analysis of swelling behavior of polymeric membranes in solutions. 2005 , 46, 8331-8339	1
1542	New local composition model for polymer solutions. 2005 , 46, 11517-11526	13
1541	An extension of the group contribution method for estimating thermodynamic and transport properties part II. Polyatomic gases (F2, Cl2, CS2, H2S, NO and N2O). 2005 , 22, 268-275	5
1540	An extension of the group contribution method for estimating thermodynamic and transport properties. Part III. Noble gases. 2005 , 22, 949-959	4
1539	A modified UNIFAC model for the prediction of phase equilibrium for polymer solutions. 2005 , 43, 2541-2547	4
1538	New free-volume-related activity model for polymer solutions. 2005 , 43, 3299-3307	1

1537	Development of the computer software. 2005 , 6, 90-96		4
1536	Homogeneous nucleation of n-nonane and n-propanol mixtures: a comparison of classical nucleation theory and experiments. 2005 , 123, 244502		21
1535	Thermodynamics of binary mixtures with strongly negative deviations from Raoult's Law. X. linear alkanoate + CHCl3 or + 1,1,2,2-tetrachloroethane. 2005 , 43, 317-332		4
1534	Theoretical prediction of the coordination number, local composition, and pressure-volume-temperature properties of square-well and square-shoulder fluids. 2005 , 123, 244505		8
1533	PLANTWIDE CONTROL STUDY OF A VINYL ACETATE MONOMER PROCESS DESIGN. 2005 , 192, 1243-125	57	24
1532	Synthesis of esters by immobilized-lipase-catalyzed condensation reaction of sugars and fatty acids in water-miscible organic solvent. 2005 , 99, 87-94		53
1531	Automated multiple headspace extraction procedure: adsorption modeling and determination of air-to-water partition coefficients. 2005 , 77, 3053-9		8
1530	Simplification of the representation of the organic component of atmospheric particulates. 2005 , 130, 341-62; discussion 363-86, 519-24		106
1529	Correlation and Prediction of Environmental Properties of Alcohol Ethoxylate Surfactants Using the UNIFAC Method. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 7255-7261	3.9	12
1528	Prediction of the McAllister Model Parameters by Using the Group-Contribution Method: n-Alkane Liquid Systems. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 9962-9968	3.9	8
1527	Experimental and Predicted Vaporlliquid Equilibrium for Cyclic Ethers with 1-Chloropentane. <i>Industrial & Discourse Engineering Chemistry Research</i> , 2005 , 44, 6981-6988	3.9	13
1526	Estimating partition coefficients for fuel-water systems: developing linear solvation energy relationships using linear solvent strength theory to handle mixtures. 2005 , 39, 2702-10		14
1525	New Experimental Results for the Vaporliquid Equilibrium of the Binary System (Trioxane + Water) and the Ternary System (Formaldehyde + Trioxane + Water). <i>Journal of Chemical & Engineering Data</i> , 2005 , 50, 1218-1223	2.8	25
1524	Hygroscopicity of water-soluble organic compounds in atmospheric aerosols: amino acids and biomass burning derived organic species. 2005 , 39, 1555-62		151
1523	Measurement and Development of Solubility Correlations for Tritolylamine in Twelve Organic Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 970-976	3.9	16
1522	Viscosity Calculations on the Basis of Eyring's Absolute Reaction Rate Theory and COSMOSPACE. <i>Industrial & Discourse Chemistry Research</i> , 2005 , 44, 8428-8435	3.9	20
1521	Liquid Liquid Equilibria of Water + Acetic Acid + Dimethyl Glutarate Ternary System. <i>Journal of Chemical & Ch</i>	2.8	13
1520	Binary Vaporliquid Equilibrium Predictions with COSMOSPACE. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 8873-8882	3.9	4

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1519	Measurement and Prediction of Solubility of Four Arylamine Molecules in Benzene, Hexane, and Methanol. <i>Journal of Chemical & Engineering Data</i> , 2005 , 50, 1794-1800	2.8	6
1518	Effect of Nonidealities in Perfume Mixtures Using the Perfumery Ternary Diagrams (PTD) Concept. <i>Industrial & Diagrams (PTD) Concept.</i>	3.9	13
1517	Experimental (Solid + Liquid) and (Liquid + Liquid) Equilibria and Excess Molar Volume of Alkanol + Acetonitrile, Propanenitrile, and Butanenitrile Mixtures <i>Journal of Chemical & Data</i> , 2005 , 50, 2035-2044	2.8	18
1516	Solvent Extraction of Ethanol from Aqueous Solutions. II. Linear, Branched, and Ring-Containing Alcohol Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 6797-6803	3.9	21
1515	Biodegradation of petroleum hydrocarbons in an immobilized cell airlift bioreactor. 2005 , 39, 3704-14		47
1514	Determination of Ion-Specific NRTL Parameters for Predicting Phase Equilibria in Aqueous Multielectrolyte Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 3289-3297	3.9	14
1513	Control of Product Quality in Batch Crystallization of Pharmaceuticals and Fine Chemicals. Part 1: Design of the Crystallization Process and the Effect of Solvent. 2005 , 9, 858-872		49
1512	A New Decomposition-Based Computer-Aided Molecular/Mixture Design Methodology for the Design of Optimal Solvents and Solvent Mixtures. <i>Industrial & Design Selection Chemistry Research</i> , 2005 , 44, 4785-4797	3.9	150
1511	Extension of Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 8909-8921	3.9	27
1510	Revision of MOSCED Parameters and Extension to Solid Solubility Calculations. <i>Industrial & Engineering Chemistry Research</i> , 2005 , 44, 4075-4083	3.9	66
1509	Thermodynamics of Binary Mixtures Containing a Very Strongly Polar Compound. 7. Isothermal VLE Measurements for NMP + 2-Propanol or + 2-Butanol Systems. DISQUAC and ERAS Characterization of NMP or N,N-Dialkylamide + 2-Alkanol Mixtures. Comparison with Results from Dortmund	3.9	20
1508	Phase Equilibrium in Formaldehyde Containing Multicomponent Mixtures: Experimental Results for Fluid Phase Equilibria of (Formaldehyde + (Water or Methanol) + Methylal)) and (Formaldehyde + Water + Methanol + Methylal) and Comparison with Predictions. <i>Industrial & Description</i> (Methylal) and Comparison with Predictions.	3.9	2
1507	Phase Equilibrium in Formaldehyde Containing Multicomponent Mixtures: Experimental Results for Fluid Phase Equilibria of (Formaldehyde + (Water or Methanol) + Methylal)) and (Formaldehyde + Water + Methanol + Methylal) and Comparison with Predictions. <i>Industrial & Descriptions</i>	3.9	55
1506	Chemistry Research, 2006 , 45, 5155-5164 Thermodynamic models of aqueous solutions containing inorganic electrolytes and dicarboxylic acids at 298.15 K. 1. The acids as nondissociating components. 2006 , 110, 5692-717		126
1505	Solubilization of polymers by ionic liquids. 2006 , 16, 4281		214
1504	Measurement and correlation of liquidliquid equilibria of methanol + 2-butanone + n-alkanes (C10 I I12) ternary mixtures. 2006 , 44, 293-301		1
1503	Synthesis of reactive separation processes. 2006 , 7-94		3
1502	Prediction of Diffusion Coefficients in Liquid Systems. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 1822-1828	3.9	45

1501	A New Activity Model for Polymer Solutions in the Frame of Lattice Theory. <i>Industrial & amp; Engineering Chemistry Research</i> , 2006 , 45, 365-371	3.9	3
1500	Liquid[liquid Equilibria for the Ternary System Methyl Isobutyl Ketone + Water + Hydroquinone. Journal of Chemical & Data, 2006, 51, 2107-2109	2.8	51
1499	Pilot-Plant Technical Assessment of Wet Flue Gas Desulfurization Using Limestone <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 6093-6093	3.9	3
1498	Measurement and Prediction of Solubility of Paracetamol in WaterBopropanol Solution. Part 2. Prediction. 2006 , 10, 1110-1118		55
1497	An Alternative Approach to Nonrandomness in Solution Thermodynamics. <i>Industrial & amp;</i> Engineering Chemistry Research, 2006 , 45, 7264-7274	3.9	9
1496	Equilibrium phase diagrams of aqueous mixtures of malonic acid and sulfate/ammonium salts. 2006 , 110, 12158-65		28
1495	Vapor Liquid Equilibrium for Six Binary Systems of C4-Hydrocarbons + 2-Propanone. <i>Journal of Chemical & Chemi</i>	2.8	15
1494	Vaporlliquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) (1) + Acetonitrile (2) Systems at 93.32 kPa. <i>Journal of Chemical & Data</i> , 2006, 51, 1536-7	1340	11
1493	Thermodynamic models of aqueous solutions containing inorganic electrolytes and dicarboxylic acids at 298.15 K. 2. Systems including dissociation equilibria. 2006 , 110, 5718-34		102
1492	Evaluation of Three Prediction Methods for Partitioning Coefficients of Organic Solutes between a Long-Chain Aliphatic Alcohol and the Gas Phase as a Function of Temperature. <i>Journal of Chemical & Engineering Data</i> , 2006 , 51, 330-337	2.8	4
1491	Measurements of Quaternary Liquid Liquid Equilibrium for Water + Acetic Acid + Propionic Acid + Solvent (Butyronitrile, Benzyl Acetate, or Methyl Isobutyl Ketone) at 298.15 K. <i>Journal of Chemical & Engineering Data</i> , 2006 , 51, 1066-1069	2.8	14
1490	Solubilities at High Dilution of Toluene, Ethylbenzene, 1,2,4-Trimethylbenzene, and Hexane in Di-2-ethylhexyl, Diisoheptyl, and Diisononyl Phthalates. <i>Journal of Chemical & Discounty Engineering Data</i> , 2006 , 51, 1212-1215	2.8	34
1489	Solvent Design Using a Quantum Mechanical Continuum Solvation Model. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 1128-1140	3.9	16
1488	Modification of UNIFAC parameter table Revision 5 for representation of aqueous solubility and 1-octanol/water partition coefficient for POPs. 2006 , 63, 698-706		3
1487	Liquid Diquid Phase Equilibrium in Glycerol Methanol Methyl Oleate and Glycerol Monoolein Methyl Oleate Ternary Systems. <i>Industrial & amp; Engineering Chemistry Research</i> , 2006 , 45, 3693-3696	3.9	96
1486	Further Development of Modified UNIFAC (Dortmund): Revision and Extension 5. <i>Industrial & Engineering Chemistry Research</i> , 2006 , 45, 7924-7933	3.9	114
1485	Liquid - liquid equilibria of the water + butyric acid + decanol ternary system. 2006 , 23, 365-374		11
1484	Effect of Cosolvents on Toxaphene Aqueous Solubility. 2006 , 3, 111		6

1483 Verfahrenstechnische Grundlagen zu Stoffaustausch und W\[\text{Ime} \] Bertragung. 187-301

1482	The effect of physical and chemical aerosol properties on warm cloud droplet activation. 2006 , 6, 2593-	2649	571
1481	Correlation of vapor - liquid equilibrium data for acetic acid - isopropanol - water - isopropyl acetate mixtures. 2006 , 23, 93-103		7
1480	Analysis of solvent-free ethyl oleate enzymatic synthesis at equilibrium conditions. 2006 , 38, 914-920		21
1479	The partial solubility parameters: An equation-of-state approach. Fluid Phase Equilibria, 2006, 240, 144-	1 <i>5.</i> 45	65
1478	Applied thermodynamics: A new frontier for biotechnology. Fluid Phase Equilibria, 2006, 241, 205-215	2.5	46
1477	Toward development of activity coefficient models for process and product design of complex chemical systems. <i>Fluid Phase Equilibria</i> , 2006 , 241, 103-112	2.5	31
1476	LiquidIIquid equilibrium data for water+ethanol+trans-decalin: Measurement and predication. <i>Fluid Phase Equilibria</i> , 2006 , 243, 45-50	2.5	14
1475	Prediction of phase equilibria for mixtures containing water, hydrocarbons and alcohols at high temperatures and pressures by cubic equation of state with GE type mixing rule based on COSMO-RS. <i>Fluid Phase Equilibria</i> , 2006 , 243, 183-192	2.5	25
1474	Applications of the simplified perturbed-chain SAFT equation of state using an extended parameter table. <i>Fluid Phase Equilibria</i> , 2006 , 248, 29-43	2.5	120
1473	Infinite dilution activity coefficients, specific retention volumes and solvation thermodynamics of hydrocarbons in C78H158 branched alkane solvent. <i>Fluid Phase Equilibria</i> , 2006 , 248, 78-88	2.5	4
1472	(Liquid+liquid) equilibria of (water+propionic acid+methyl isoamyl ketone or diisobutyl ketone or ethyl isoamyl keton) at T=298.2K. <i>Fluid Phase Equilibria</i> , 2006 , 250, 70-75	2.5	17
1471	A computer-aided molecular design framework for crystallization solvent design. 2006 , 61, 1247-1260		124
1470	A conformal solution theory for the energy landscape and glass transition of mixtures. <i>Fluid Phase Equilibria</i> , 2006 , 241, 147-154	2.5	16
1469	(Liquid + liquid) equilibria of (water + 1-propanol + solvent) at T=298.2K. Fluid Phase Equilibria, 2006 , 239, 156-160	2.5	19
1468	Chemical equilibria of multiple-reaction systems from reaction ensemble Monte Carlo simulation and a predictive equation of state: Combined hydrogenation of ethylene and propylene. <i>Fluid Phase Equilibria</i> , 2006 , 242, 189-203	2.5	12
1467	Prediction of phase equilibria with strong electrolytes with the help of the volume translated Peng-Robinson group contribution equation of state (VTPR). <i>Fluid Phase Equilibria</i> , 2006 , 246, 111-118	2.5	19
1466	LiquidIquid equilibria of ternary systems (water + carboxylic acid + cumene) at 298.15 K. <i>Fluid Phase Equilibria</i> , 2006 , 248, 24-28	2.5	20

1465	Thermodynamics of isomeric hexynes+MTBE binary mixtures. <i>Fluid Phase Equilibria</i> , 2006 , 248, 181-190 2.	5	13
1464	The concept of associated solutions in historical development. Part 1. The 1884 1984 period. 2006 , 128, 1-31		17
1463	Extension of TI th Psi function from gas-solid to liquid-solid equilibria and application to reversed-phase liquid chromatography systems. 2006 , 299, 136-54		3
1462	(Liquid+liquid) equilibria of the (water+acetic acid+dibasic esters mixture) system. 2006 , 38, 1669-1674		12
1461	(Liquid+liquid) equilibria of (water+propionic acid+alcohol) ternary systems. 2006, 38, 1503-1509		25
1460	Thermodynamics of organic mixtures containing amines. 2006 , 441, 53-68		35
1459	Excess molar volumes of N,N-dimethylformamide + 2-pentanone + alkan-1-ols mixed solvent systems at 303.15 K. 2006 , 443, 62-71		37
1458	Structural and electrostatic properties of atoms and functional groups using AIM theory: Saturated organics with one electronegative atom. 2006 , 770, 31-44		5
1457	Computer-Aided Modelling of Short-Path Evaporation for Chemical Product Purification, Analysis and Design. 2006 , 84, 583-594		13
1456	Predicting infinite dilution activity coefficients of organic compounds in water by quantum-connectivity descriptors. 2006 , 20, 539-48		11
1455	Characterization and solubility measurement and prediction of selected arylamines in hexane, methanol and benzene. 2006 , 61, 2590-2598		6
1454	Thermodynamic equations of state from molecular solvation. <i>Fluid Phase Equilibria</i> , 2006 , 245, 185-192 2.	5	10
1453	Comparison of two modeling approaches for describing intra-diffusion in liquid Lennardlones mixtures containing a self-associating component. <i>Fluid Phase Equilibria</i> , 2006 , 245, 140-148	5	6
1452	Investigation of different activity coefficient models in thermodynamic modeling of wax precipitation. <i>Fluid Phase Equilibria</i> , 2006 , 248, 7-18	5	20
1451	Liquid phase equilibria of (water + propionic acid + oleyl alcohol) ternary system at several temperatures. <i>Fluid Phase Equilibria</i> , 2006 , 250, 59-63	5	30
1450	(Liquid + liquid) equilibria of the (water + butyric acid + dodecanol) ternary system. 2006 , 38, 696-700		25
1449	Phase equilibria of liquid (water + butyric acid + oleyl alcohol) ternary system. 2006 , 38, 1634-1639		26
1448	Prediction of activity coefficients in liquid aerosol particles containing organic compounds, dissolved inorganic salts, and waterPart 3: Organic compounds, water, and ionic constituents by consideration of short-, mid-, and long-range effects using X-UNIFAC.3. 2006 , 40, 6437-6452		31

(2007-2006)

1447	Prediction of activity coefficients in liquid aerosol particles containing organic compounds, dissolved inorganic salts, and waterPart 1: Organic compounds and water by consideration of short- and long-range effects using X-UNIFAC.1. 2006 , 40, 6410-6421	22
1446	Prediction of activity coefficients in liquid aerosol particles containing organic compounds, dissolved inorganic salts, and waterPart 2: Consideration of phase separation effects by an X-UNIFAC model. 2006 , 40, 6422-6436	62
1445	Effects of initial saturation on properties modification and displacement of tetrachloroethene with aqueous isobutanol. 2006 , 88, 69-91	1
1444	Practical Methodology for Distillation Design using a Miniplant. 2006 , 29, 104-112	3
1443	Thermodynamic modeling of activity coefficient and prediction of solubility: Part 1. Predictive models. 2006 , 95, 790-7	10
1442	Determination of solubility profiles of eflucimibe polymorphs: experimental and modeling. 2006 , 95, 871-82	7
1441	Thermodynamic modeling of activity coefficient and prediction of solubility: Part 2. Semipredictive or semiempirical models. 2006 , 95, 798-809	31
1440	Simple Approach for Quantifying the Thermodynamic Potential of Polymer Polymer Adhesion. 2006 , 82, 121-133	10
1439	On planar laser-induced fluorescence with multi-component fuel and tracer design for quantitative determination of fuel concentration in internal combustion engines. 2007 , 221, 713-724	13
1438	Solvent design for crystallization of pharmaceutical products. 2007 , 23, 115-147	1
1437	Chapter 5.4 Modelling seasonal changes of aerosol compositions over Belgium and Europe. 2007 , 6, 514-522	2
		²
	Chapter 5.4 Modelling seasonal changes of aerosol compositions over Belgium and Europe. 2007 , 6, 514-522 Surface tensions of multi-component mixed inorganic/organic aqueous systems of atmospheric significance: measurements, model predictions and importance for cloud activation predictions.	
1436	Chapter 5.4 Modelling seasonal changes of aerosol compositions over Belgium and Europe. 2007 , 6, 514-522 Surface tensions of multi-component mixed inorganic/organic aqueous systems of atmospheric significance: measurements, model predictions and importance for cloud activation predictions. 2007 , 7, 2371-2398 Closure study between chemical composition and hygroscopic growth of aerosol particles during	76
1436 1435	Chapter 5.4 Modelling seasonal changes of aerosol compositions over Belgium and Europe. 2007 , 6, 514-522 Surface tensions of multi-component mixed inorganic/organic aqueous systems of atmospheric significance: measurements, model predictions and importance for cloud activation predictions. 2007 , 7, 2371-2398 Closure study between chemical composition and hygroscopic growth of aerosol particles during TORCH2. 2007 , 7, 6131-6144 Cloud condensation nucleus (CCN) behavior of organic aerosol particles generated by atomization	76 206
1436 1435 1434	Chapter 5.4 Modelling seasonal changes of aerosol compositions over Belgium and Europe. 2007, 6, 514-522 Surface tensions of multi-component mixed inorganic/organic aqueous systems of atmospheric significance: measurements, model predictions and importance for cloud activation predictions. 2007, 7, 2371-2398 Closure study between chemical composition and hygroscopic growth of aerosol particles during TORCH2. 2007, 7, 6131-6144 Cloud condensation nucleus (CCN) behavior of organic aerosol particles generated by atomization of water and methanol solutions. 2007, 7, 2949-2971 Azeotropic data for the systems formed by representatives of the homologous series of alkanes	76 206 42
1436 1435 1434 1433	Chapter 5.4 Modelling seasonal changes of aerosol compositions over Belgium and Europe. 2007, 6, 514-522 Surface tensions of multi-component mixed inorganic/organic aqueous systems of atmospheric significance: measurements, model predictions and importance for cloud activation predictions. 2007, 7, 2371-2398 Closure study between chemical composition and hygroscopic growth of aerosol particles during TORCH2. 2007, 7, 6131-6144 Cloud condensation nucleus (CCN) behavior of organic aerosol particles generated by atomization of water and methanol solutions. 2007, 7, 2949-2971 Azeotropic data for the systems formed by representatives of the homologous series of alkanes and alcohols. 2007, 26, 595-610 Physicochemical properties of selected polybrominated diphenyl ethers and extension of the	76 206 42 11

1429	Refinement of COSMOBAC and the Applications. <i>Industrial & Engineering Chemistry Research</i> , 2007 , 46, 7275-7288	3.9	148
1428	A group contribution method for associating chain molecules based on the statistical associating fluid theory (SAFT-gamma). 2007 , 127, 234903		195
1427	A general local composition and coordination number model for square-well fluids with variable well width and diameter ratio. 2007 , 105, 1019-1037		3
1426	LiquidIquid equilibrium for system corn oil + oleic acid + ethanol + water. 2007 , 45, 623-629		7
1425	Molecular solvation in water-methanol and water-sorbitol mixtures: the roles of preferential hydration, hydrophobicity, and the equation of state. 2007 , 111, 4467-76		23
1424	Liquidliquid Equilibria of the Ternary System Water + Acetic Acid + Methyltert-Butyl Ether. Journal of Chemical & Data, 2007, 52, 789-793	2.8	20
1423	Phase equilibrium of binary mixtures of cyclic ethers + chlorobutane isomers: experimental measurements and SAFT-VR modeling. 2007 , 111, 9588-97		16
1422	Adipic and malonic acid aqueous solutions: surface tensions and saturation vapor pressures. 2007 , 111, 12995-3002		53
1421	Liquid Liquid Liquid Equilibria of (Water + Acetic Acid + Diethyl Succinate or Diethyl Glutarate or Diethyl Adipate) Ternary Systems. <i>Journal of Chemical & Chemical</i>	2.8	33
1420	Viscosities of Fatty Mixtures: Experimental Data and Prediction. <i>Journal of Chemical & Engineering Data</i> , 2007 , 52, 2000-2006	2.8	25
1419	Determination of evaporation rates and vapor pressures of very low volatility compounds: a study of the C4-C10 and C12 dicarboxylic acids. 2007 , 111, 3099-109		86
1418	Ternary and Quaternary Liquid + Liquid Equilibria for Systems of (Water + Toluene +m-Xylene + Phenol). <i>Journal of Chemical & Engineering Data</i> , 2007 , 52, 180-183	2.8	15
1417	Vaporliquid Equilibrium Data for the Binary Methyl Esters (Butyrate, Pentanoate, and Hexanoate) (1) + Propanenitrile (2) Systems at 93.32 kPa. <i>Journal of Chemical & Data</i> , 2007, 52, 871-	87 5	15
1416	Making Equation of State Models Predictive P art 3: Improved Treatment of Multipolar Interactions in a PC-SAFT Based Equation of State 2007 , 111, 15533-15543		16
1415	Thermodynamic properties of malonic, succinic, and glutaric acids: evaporation rates and saturation vapor pressures. 2007 , 41, 3926-33		35
1414	Vaporliquid Equilibria Predictions for New Refrigerant Mixtures Based on Group Contribution Theory. <i>Industrial & Engineering Chemistry Research</i> , 2007 , 46, 9274-9284	3.9	21
1413	Liquid Liquid Liquid Equilibria for Ternary Systems of Water + Formic Acid + Dibasic Esters. <i>Journal of Chemical & Chemi</i>	2.8	34
1412	Liquid Liquid Equilibrium for Systems of (Corn Oil + Oleic Acid + Methanol or Ethanol) at (303.15 and 313.15) K. <i>Journal of Chemical & Data</i> , 2007, 52, 910-914	2.8	21

1411	A Model for Estimating Vapor Pressures of Commingled Ethanol Fuels. 2007 ,		9
1410	Modeling solubilities of sugars in alcohols based on original experimental data. <i>AICHE Journal</i> , 2007 , 53, 2411-2418	3.6	50
1409	Vapourlīquid equilibrium for the systems butane+methanol, +2-propanol, +1-butanol, +2-butanol, +2-methyl-2-propanol at 364.5K. <i>Fluid Phase Equilibria</i> , 2007 , 254, 49-59	2.5	18
1408	Solubility and local structure around a dilute solute molecule in an aqueous solvent: From gases to biomolecules. <i>Fluid Phase Equilibria</i> , 2007 , 260, 126-134	2.5	6
1407	Vapour l Iquid equilibrium of cyclic ethers with 1-chlorohexane: Experimental results and UNIFAC predictions. <i>Fluid Phase Equilibria</i> , 2007 , 257, 70-77	2.5	9
1406	Making equation of state models predictive. <i>Fluid Phase Equilibria</i> , 2007 , 258, 16-28	2.5	23
1405	Liquid II quid equilibria for the quaternary system methyl isobutyl ketone Water II henol II ydroquinone. Fluid Phase Equilibria, 2007, 258, 73-77	2.5	42
1404	Sorption and diffusion measurements in ternary polymerBolventBolvent systems by means of a magnetic suspension balanceExperimental methods and correlations with a modified FloryHuggins and free-volume theory. 2007 , 62, 2254-2266		44
1403	Hydrogen-bond networks in linear, branched and tertiary alcohols. 2007, 62, 3019-3031		27
1402	Thermodynamics of adsorption of binary aqueous organic liquid mixtures on a RPLC adsorbent. 2007 , 1155, 85-99		60
1401	Influence of preferential adsorption of mobile phase on retention behavior of amino acids on the teicoplanin chiral selector. 2007 , 1173, 58-70		20
1400	Extension of the group-contribution lattice-fluid equation of state. Fluid Phase Equilibria, 2007, 260, 135	21 4 5	9
1399	Application of force field in Gibbs ensemble lattice statistics to model vapor/liquid equilibria. <i>Fluid Phase Equilibria</i> , 2007 , 252, 175-188	2.5	3
1398	A simplified approach to vaporliquid equilibria calculations with the group-contribution lattice-fluid equation of state. <i>Fluid Phase Equilibria</i> , 2007 , 259, 116-122	2.5	3
1397	Effect of temperature gradient on Marangoni condensation heat transfer for ethanol water mixtures. 2007 , 33, 935-947		24
1396	Solubility analysis of buspirone hydrochloride polymorphs: measurements and prediction. 2007 , 338, 55-63		31
1395	Erratum to The concept of associated solutions in historical development: Part 1. The 1884 1984 period [J. Mol. Liq. 128 (2006) 1 1 2 1 2 1 2 1 2 1 2 2 1 2 2 1 2 2 1 2		8
1394	Analysis of methanol extraction from aqueous solution by n-hexane: Equilibrium diagrams as a function of temperature. 2007 , 130, 52-58		9

1393	(Liquid+liquid) equilibria of (water+propionic acid+dipropyl ether or diisopropyl ether) at T=298.2K. 2007 , 39, 123-127		24
1392	(Liquid+liquid) equilibria of (water+butyric acid+esters) ternary systems. 2007 , 39, 1279-1285		25
1391	(Liquid+liquid) equilibria of (water+propionic acid+dibasic esters) ternary systems. 2007 , 39, 1493-1499		21
1390	Use of analytical solutions of groups (ASOG) contribution method to predict water activity in solutions of sugars, polyols and urea. 2007 , 29, 331-338		10
1389	A Modification of £ n SRK Equation of State and Vapor-Liquid Equilibria Prediction. 2007 , 15, 102-109		10
1388	Solid-Liquid Equilibria of trans-1,2-Cyclohexanediol+Butyl Acetate+ Water Ternary System. 2007 , 15, 449-452		5
1387	Prediction of polycyclic aromatic hydrocarbon solubilities in benzene. 2007 , 2, 144-150		1
1386	Measurement and Prediction of Oxygen Solubility in Toluene at Temperatures from 298.45 K to 393.15 K and Pressures up to 1.0 MPa. <i>Journal of Chemical & Engineering Data</i> , 2007 , 52, 2339-2344 2.5	8	38
1385	Glycerolysis of Fatty Acid Methyl Esters: 1. Investigations in a Batch Reactor. 2007 , 84, 83-90		15
1384	Prediction of the Partition Coefficient for Acetic Acid in a Two-Phase System Soybean Oil-Water. 2007 , 84, 669-674		6
1383	Phase equilibria of water + 1-propanol + solvent (n-amyl acetate, cyclohexanol, and cyclohexyl acetate) at T = 298.2 K. <i>Fluid Phase Equilibria</i> , 2007 , 253, 61-66	5	20
1382	Prediction of vaporIIquid equilibria using reconstructionLearning neural network method. Fluid Phase Equilibria, 2007, 257, 169-172	5	9
1381	Classical and recent free-volume models for polymer solutions: A comparative evaluation. <i>Fluid Phase Equilibria</i> , 2007 , 257, 63-69	5	16
1380	Measurement of vaporllquid equilibria (VLE) and excess enthalpies (HE) of binary systems with 1-alkyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide and prediction of these properties 2.1 and Ausing modified UNIFAC (Dortmund). Fluid Phase Equilibria, 2007, 258, 168-178	5	115
1379	Estimations of the viscosities of binary mixtures with different equations of state and mixing rules. 2007 , 38, 1-19		8
1378	(Liquid + liquid) equilibria of (water + butyric acid + dibasic esters) ternary systems. 2007 , 39, 284-290		32
1377	(Liquid+liquid) equilibria of (water+propionic acid+diethyl succinate or diethyl glutarate or diethyl adipate) ternary systems. 2007 , 39, 1463-1469		38
1376	Molar excess enthalpy for various {alkanolamine (1)+water (2)} systems at T=(298.15, 313.15, and 323.15)K. 2007 , 39, 1439-1451		19

(2008-2008)

1375	Liquid I quid equilibria of water+2,3-butanediol+ethyl acetate at several temperatures. Fluid Phase Equilibria, 2008 , 266, 42-46	2.5	21	
1374	LiquidIquid equilibria of the systems isobutyl acetate+isobutyl alcohol+water and isobutyl acetate+isobutyl alcohol+glycerol at different temperatures. <i>Fluid Phase Equilibria</i> , 2008 , 265, 122-128	2.5	11	
1373	Quantitative solubility relationships and the effect of water uptake in triglyceride/monoglyceride microemulsions. 2008 , 25, 1158-74		15	
1372	Extension of the EUROS Integrated Air Quality Model to Fine Particulate Matter by Coupling to CACM/MADRID 2. 2008 , 13, 431-437		3	
1371	Kinematic Viscosities for Ether + Alkane Mixtures: Experimental Results and UNIFAC-VISCO Parameters. 2008 , 29, 457-467		18	
1370	Experimental study on the condensation of ethanolWater mixtures on vertical tube. 2008, 44, 607-616		21	
1369	Characterization of Mixtures Part 1: Prediction of Infinite-Dilution Activity Coefficients Using Neural Network-Based QSPR Models. 2008 , 27, 1346-1361		19	
1368	The effect of solvents on the rate of catalytic hydrogenation of 6-ethyl-1,2,3,4-tetrahydroanthracene-9,10-dione. 2008 , 40, 240-252		13	
1367	Measurement and Prediction of the Solubility of Stearic Acid Polymorphs by the UNIQUAC Equation. 2008 , 82, 335-342		27	
1366	On Criteria for Occurrence of Azeotropes in Isothermal and Isobaric Binary Systems. 2008 , 83, 667-674		10	
1365	Elastic effects on solubility in semicrystalline polymers. 2008, 107, 138-146		20	
1364	Development of a mathematical model for studying bioethanolWater separation using hydrophilic polyetherimide membrane. 2008 , 107, 2256-2265		8	
1363	A semi-empirical cell voltage model for polymer electrolyte/methanol systems: Applicability of the group contribution method. 2008 , 110, 3186-3194			
1362	Illustrating computational solvent screening: Prediction of standard Gibbs energies of reaction in solution. <i>AICHE Journal</i> , 2008 , 54, 2729-2734	3.6	16	
1361	Thermodynamics of Aqueous Systems. 141-191		1	
1360	Phase separation in aqueous two-phase systems containing poly(ethylene glycol) and magnesium sulphate at different temperatures. 2008 , 40, 573-579		12	
1359	Isobaric (vapour + liquid + liquid) equilibrium data for (di-n-propyl ether + n-propyl alcohol + water) and (diisopropyl ether + isopropyl alcohol + water) systems at 100 kPa. 2008 , 40, 867-873		21	
1358	Mixing thermodynamic properties of 1-butyl-4-methylpyridinium tetrafluoroborate [b4mpy][BF4] with water and with an alkan-1ol (methanol to pentanol). 2008 , 40, 1087-1094		47	

1357	Isothermal (vapour + liquid) equilibrium of (cyclic ethers + chlorohexane) mixtures: Experimental results and SAFT modelling. 2008 , 40, 1253-1260		6
1356	Evaluation of (vapor + liquid) equilibria for the binary systems (1-octanol + cyclohexane) and (1-octanol + n-hexane), at low alcohol compositions. 2008 , 40, 1617-1620		2
1355	Determination of the activity of a molecular solute in saturated solution. 2008, 40, 1684-1692		40
1354	Phase equilibria of the ternary system vinyl acetate/(R,S)-1-phenylethanol/carbon dioxide at high pressure conditions. <i>Fluid Phase Equilibria</i> , 2008 , 267, 104-112	2.5	4
1353	Study of liquid IIquid equilibrium of the systems isobutyl acetate+acetic acid+water and isobutyl alcohol+acetic acid+water at different temperatures. <i>Fluid Phase Equilibria</i> , 2008 , 271, 76-81	2.5	29
1352	Multiphase equilibria for mixtures containing water, acetic acid, propionic acid, methyl acetate and methyl propionate. <i>Fluid Phase Equilibria</i> , 2008 , 271, 69-75	2.5	9
1351	Application of the group contribution concept to Kihara potential for estimating thermodynamic and transport properties. <i>Fluid Phase Equilibria</i> , 2008 , 271, 53-68	2.5	5
1350	Phase equilibria of (water+levunilic acid+alcohol) ternary systems. Fluid Phase Equilibria, 2008, 273, 21-2	. 6 .5	30
1349	Computer aided aroma design IMolecular knowledge framework. 2008 , 47, 1902-1911		16
1348	Modeling of phase equilibrium of binary mixtures composed by polystyrene and chlorofluorocarbons, hydrochlorofluorocarbons, hydrofluorocarbons and supercritical fluids using cubic and non-cubic equations of state. 2008 , 45, 134-145		14
1347	Applying UNIFAC-based models to predict the solubility of solids in subcritical water. 2008 , 46, 245-251		22
1346	Prediction of vaporliquid equilibria for supercritical alcohol+fatty acid ester systems by SRK equation of state with WongBandler mixing rule based on COSMO theory. 2008 , 46, 4-9		18
1345	Thermodynamics of mixtures containing amines: VII. Systems containing dimethyl or trimethylpyridines. 2008 , 467, 30-43		14
1344	LiquidIquid equilibria of water+2,3-butanediol+1-butanol at T=298.15K, T=308.15K and T=318.15K. <i>Fluid Phase Equilibria</i> , 2008 , 265, 1-6	2.5	23
1343	Vapourliquid equilibria of aroma compounds in hydroalcoholic solutions: Measurements with a recirculation method and modelling with the NRTL and COSMO-SAC approaches. <i>Fluid Phase Equilibria</i> , 2008 , 265, 139-154	2.5	29
1342	A generalisation of the SAFT-數roup contribution method for groups comprising multiple spherical segments. <i>Fluid Phase Equilibria</i> , 2008 , 274, 85-104	2.5	116
1341	A method for calculating the Gibbs energy of nonspecific solvation. 2008 , 82, 704-708		10
1340	What determines drug solubility in lipid vehicles: is it predictable?. 2008 , 60, 638-56		122

1339	Effects of organics on efflorescence relative humidity of ammonium sulfate or sodium chloride particles. 2008 , 42, 4433-4445		9
1338	Tuning the Morphology of Pharmaceutical Compounds via Model Based Solvent Selection. 2008 , 16, 465-473		9
1337	Analysis and Comparison of the Alpha Functions of SRK Equation of State. 2008 , 16, 766-771		8
1336	Vaporliquid Equilibrium for Butane + Methanol, + Ethanol, + 2-Propanol, + 2-Butanol, and + 2-Methyl-2-Propanol (TBA) at 323 K. <i>Journal of Chemical & Data</i> , 2008 , 53, 83-88	2.8	13
1335	Predictive molecular thermodynamic models for liquid solvents, solid salts, polymers, and ionic liquids. 2008 , 108, 1419-55		122
1334	HTDMA analysis of multicomponent dicarboxylic acid aerosols with comparison to UNIFAC and ZSR. 2008 , 113,		23
1333	Self-Condensation of Cyclohexanone over Ion Exchange Resin Catalysts: Kinetics and Selectivity Aspects. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 25-33	3.9	34
1332	Liquid[liquid Extraction. 2008,		9
1331	Vaporliquid Equilibrium for the cis-2-Butene + Methanol, + 2-Propanol, + 2-Butanol, + 2-Methyl-2-propanol Systems at 364.5 K. <i>Journal of Chemical & Engineering Data</i> , 2008 , 53, 1539-154	24 ⁸	5
1330	Liquid Diquid Equilibria of Mixtures Containing Methyl Acetate + Methanol + Hexane or Heptane. Journal of Chemical & Data, 2008, 53, 89-93	2.8	4
1329	Study of fuel oxygenates solubility in aqueous media as a function of temperature and tert-butyl alcohol concentration. 2008 , 71, 2098-105		17
1328	Phase Equilibria in Ternary Mixtures of Methyl Oleate, Glycerol, and Methanol. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 5157-5164	3.9	95
1327	Estimation of Physical Properties. 2008,		3
1326	Perspective for Extended Group-Contribution Methods for the Prediction of Activity Coefficients Accounting for Sterical Effects. Linking UNIFAC and the Group Vector Space Method. <i>Industrial & Company: Engineering Chemistry Research</i> , 2008 , 47, 10080-10085	3.9	
1325	Vaporlliquid Equilibrium for the Systems trans-2-Butene + Methanol, + 1-Propanol, + 2-Propanol, + 2-Butanol, and + 2-Methyl-2-propanol at 364.5 K. <i>Journal of Chemical & Chemic</i>	2.8	6
1324	Comparative thermodynamic studies of aqueous glutaric acid, ammonium sulfate and sodium chloride aerosol at high humidity. 2008 , 112, 9413-22		49
1323	Prediction of Partition Coefficients of Benzothiophene and Benzothiophene 1,1-Dioxide in Octane/Acetonitrile System Using COSMO Theory. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 3247-3252	3.9	6
1322	Measurement and Correlation of Solubilities of trans-Resveratrol in Ethanol + Water and Acetone + Water Mixed Solvents at Different Temperatures. <i>Journal of Chemical & Different Temperatures</i> . 2008, 53, 2562-2566	2.8	21

1321	Vaporliquid Equilibrium for 1-Butene + Methanol, + 1-Propanol, + 2-Propanol, + 2-Butanol, and 2-Methyl-2-propanol (TBA) at 364.5 K. <i>Journal of Chemical & Engineering Data</i> , 2008 , 53, 1829-1835	2.8	6
1320	Phase Equilibrium of Water + Formic Acid + Acetic Acid + Solvent (Amyl Acetate or Diisobutyl Ketone or Diisopropyl Ether) Quaternary Liquid Systems. <i>Journal of Chemical & Data</i> , 2008, 53, 1607-1611	2.8	7
1319	Reaction from Dimethyl Carbonate (DMC) to Diphenyl Carbonate (DPC). 2. Kinetics of the Reactions from DMC via Methyl Phenyl Carbonate to DPC. <i>Industrial & December 2008</i> , 47, 9862-9870	3.9	28
1318	Butadiene Purification Using Polar Solvents. Analysis of Solution Nonideality Using Data and Estimation Methods. <i>Industrial & Estimation Methods</i> . <i>Industrial & Industrial &</i>	3.9	16
1317	Vaporliquid Equilibria Predictions for Alternative Working Fluids at Low and Moderate Pressures. <i>Industrial & Engineering Chemistry Research</i> , 2008 , 47, 7501-7508	3.9	9
1316	Vaporlliquid Equilibrium for 1-Butanol + 1-Butene at (318.4 and 364.5) K and Vaporlliquid Equilibrium of 1-Butanol + 2-Methylpropane, + n-Butane and 1-Butene + 2-Methylpropane at 318.4 K. <i>Journal of Chemical & Engineering Data</i> , 2008 , 53, 2454-2461	2.8	2
1315	Liquid l iquid Equilibria of (Limonene + Linalool + Ethylene Glycol or Diethylene Glycol or Triethylene Glycol or 1,2-Propylene Glycol) Ternary Systems. <i>Journal of Chemical & Data</i> , 2008 , 53, 737-741	2.8	21
1314	A heteronuclear group contribution method for associating chain molecules (SAFT- # 2008 , 25, 871-876		
1313	Effects of Vapor Pressure on Marangoni Condensation of Steam-Ethanol Mixtures. 2008 , 22, 247-253		18
1312	Fundamentals of Biocatalysis in Neat Organic Solvents. 1-24		3
1312	Fundamentals of Biocatalysis in Neat Organic Solvents. 1-24 Hydrogen Bonding and Nonrandomness in Solution Thermodynamics. 2008, 45-89		3
1311			3
1311	Hydrogen Bonding and Nonrandomness in Solution Thermodynamics. 2008 , 45-89		3
1311	Hydrogen Bonding and Nonrandomness in Solution Thermodynamics. 2008, 45-89 Thermodynamics of Fluid Phase and Chemical Equilibria. 2008, 255-392 A computationally-efficient secondary organic aerosol module for three-dimensional air quality		3
1311 1310 1309	Hydrogen Bonding and Nonrandomness in Solution Thermodynamics. 2008, 45-89 Thermodynamics of Fluid Phase and Chemical Equilibria. 2008, 255-392 A computationally-efficient secondary organic aerosol module for three-dimensional air quality models. 2008, A computationally-efficient secondary organic aerosol module for three-dimensional air quality		
1311 1310 1309	Hydrogen Bonding and Nonrandomness in Solution Thermodynamics. 2008, 45-89 Thermodynamics of Fluid Phase and Chemical Equilibria. 2008, 255-392 A computationally-efficient secondary organic aerosol module for three-dimensional air quality models. 2008, A computationally-efficient secondary organic aerosol module for three-dimensional air quality models. 2008, 8, 3985-3998 A thermodynamic model of mixed organic-inorganic aerosols to predict activity coefficients. 2008, 8, 4559-4593		4
1311 1310 1309 1308 1307	Hydrogen Bonding and Nonrandomness in Solution Thermodynamics. 2008, 45-89 Thermodynamics of Fluid Phase and Chemical Equilibria. 2008, 255-392 A computationally-efficient secondary organic aerosol module for three-dimensional air quality models. 2008, A computationally-efficient secondary organic aerosol module for three-dimensional air quality models. 2008, 8, 3985-3998 A thermodynamic model of mixed organic-inorganic aerosols to predict activity coefficients. 2008, 8, 4559-4593		238

1303	. 2008,		60
1302	Factual data banks and their application to the synthesis and design of chemical processes and the development and testing of thermophysical property estimation methods. 2009 , 81, 1745-1768		15
1301	Determination of Activity Coefficients of Semi-Volatile Organic Aerosols Using the Integrated Volume Method. 2009 , 43, 838-846		12
1300	The carbon number-polarity grid: A means to manage the complexity of the mix of organic compounds when modeling atmospheric organic particulate matter. 2009 , 43, 2829-2835		86
1299	Temperature and solvent effects in the solubility of some pharmaceutical compounds: Measurements and modeling. 2009 , 37, 499-507		99
1298	Measurement and Correlation of Solubilities of Adipic Acid in Different Solvents. 2009 , 17, 473-477		32
1297	Perfumery quaternary diagrams for engineering perfumes. AICHE Journal, 2009, 55, 2171-2185	3.6	16
1296	Group contribution prediction of surface charge density distribution of molecules for COSMO-SAC. <i>AICHE Journal</i> , 2009 , 55, 3298-3300	3.6	15
1295	Multicomponent Mass Transfer Model for Supercritical Extraction: Application to Isopropyl Alcohol Production. 2009 , 32, 1384-1391		2
1294	A neural network approach to predict activity coefficients. 2009 , 87, 748-760		4
1294	A neural network approach to predict activity coefficients. 2009 , 87, 748-760 Measurement and prediction of phase diagrams of the enantiomeric 3-chloromandelic acid system. 2009 , 64, 192-197		19
	Measurement and prediction of phase diagrams of the enantiomeric 3-chloromandelic acid system.	2.5	
1293	Measurement and prediction of phase diagrams of the enantiomeric 3-chloromandelic acid system. 2009, 64, 192-197 A comparison of mixing rules for the combination of COSMO-RS and the PengRobinson equation	2.5	19
1293	Measurement and prediction of phase diagrams of the enantiomeric 3-chloromandelic acid system. 2009, 64, 192-197 A comparison of mixing rules for the combination of COSMO-RS and the PengRobinson equation of state. Fluid Phase Equilibria, 2009, 275, 105-115 Measurement and prediction of tie-line data for mixtures of (water+1-propanol+diisopropyl ether):		19
1293 1292 1291	Measurement and prediction of phase diagrams of the enantiomeric 3-chloromandelic acid system. 2009, 64, 192-197 A comparison of mixing rules for the combination of COSMO-RS and the PengRobinson equation of state. Fluid Phase Equilibria, 2009, 275, 105-115 Measurement and prediction of tie-line data for mixtures of (water+1-propanol+diisopropyl ether): LLE diagrams as a function of temperature. Fluid Phase Equilibria, 2009, 277, 126-130 Phase equilibria of (water+levulinic acid+dibasic esters) ternary systems. Fluid Phase Equilibria,	2.5	19 13 11
1293 1292 1291 1290	Measurement and prediction of phase diagrams of the enantiomeric 3-chloromandelic acid system. 2009, 64, 192-197 A comparison of mixing rules for the combination of COSMO-RS and the PengRobinson equation of state. Fluid Phase Equilibria, 2009, 275, 105-115 Measurement and prediction of tie-line data for mixtures of (water+1-propanol+diisopropyl ether): LLE diagrams as a function of temperature. Fluid Phase Equilibria, 2009, 277, 126-130 Phase equilibria of (water+levulinic acid+dibasic esters) ternary systems. Fluid Phase Equilibria, 2009, 282, 20-24	2.5	19 13 11
1293 1292 1291 1290	Measurement and prediction of phase diagrams of the enantiomeric 3-chloromandelic acid system. 2009, 64, 192-197 A comparison of mixing rules for the combination of COSMO-RS and the PengRobinson equation of state. Fluid Phase Equilibria, 2009, 275, 105-115 Measurement and prediction of tie-line data for mixtures of (water+1-propanol+diisopropyl ether): LLE diagrams as a function of temperature. Fluid Phase Equilibria, 2009, 277, 126-130 Phase equilibria of (water+levulinic acid+dibasic esters) ternary systems. Fluid Phase Equilibria, 2009, 282, 20-24 Improvement of an Entropic-FV model based on solubility parameters for prediction of vaportiquid equilibria of solventpolymer systems. Fluid Phase Equilibria, 2009, 285, 105-111 Thermodynamic consistency of Raoult® Law and Henry® Law approaches for multiphase organic	2.5	19 13 11 10 4

1285	Measurement of ternary polymer/solvent equilibrium data by vapor-phase infrared spectroscopy. Fluid Phase Equilibria, 2009 , 277, 35-41	7
1284	Application of UNIFAC models for prediction of vaporliquid and liquidliquid equilibria relevant to separation and purification processes of crude biodiesel fuel. 2009 , 88, 1472-1477	68
1283	Marangoni condensation heat transfer of water@thanol mixtures on a vertical surface with temperature gradients. 2009 , 52, 2324-2334	27
1282	HIx system thermodynamic model for hydrogen production by the Sulfur bdine cycle. 2009 , 34, 1696-1709	20
1281	Application of a group contribution equation of state for the thermodynamic modeling of the binary systems CO2¶-butyl-3-methyl imidazolium nitrate and CO2¶-hydroxy-1-propyl-3-methyl imidazolium nitrate. 2009 , 50, 112-117	31
1280	Experimental study of methane and carbon dioxide solubility in 1,4 butylene glycol at pressures up to 11 MPa and temperatures ranging from 303 to 423 K. 2009 , 51, 123-127	8
1279	Experimental and predicted excess molar enthalpies of some working pairs for absorption cycles. 2009 , 495, 72-80	7
1278	(Liquid + liquid) equilibria of (water + lactic acid + alcohol) ternary systems. 2009 , 41, 97-102	21
1277	Finitely limited group contribution correlations for boiling temperatures. 2009 , 41, 530-537	10
1276	Present status and potential of group contribution methods for process development. 2009 , 41, 731-747	71
1275	Reply to Comment on Towards the development of theoretically correct liquid activity coefficient models 12009, 41, 1314-1316	1
1274	Ionic conductivities of perfluorosulfonic acid membrane by group contribution method. 2009 , 50, 3686-3692	7
1273	Isosteric heat of adsorption in liquid-solid equilibria: theoretical determination and measurement by liquid chromatography/mass spectrometry. 2009 , 1216, 4745-51	3
1272	A computational molecular design framework for crosslinked polymer networks. 2009 , 33, 954-963	30
1271	Thermodynamic modeling of the vaporliquid equilibrium of the CO2/H2O mixture. <i>Fluid Phase Equilibria</i> , 2009 , 284, 56-63	58
1270	Modeling of polycyclic aromatic hydrocarbon SLE in aromatic solvents. 2009 , 5, 517-526	
1269	Scalable solution cocrystallization: case of carbamazepine-nicotinamide I. 2009 , 11, 501-509	84
1268	Thermodynamic Modeling and Simulation of Styrene B utadiene Rubbers (SBR) Solvent Equilibrium Staged Processes. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 7713-7723	10

(2009-2009)

1267	Calculation of Solid[liquid[Gas Equilibrium for Binary Systems Containing CO2. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 4579-4586	3.9	14	
1266	Prediction of VaporIliquid Equilibrium at High Pressure Using a New Excess Free Energy Mixing Rule Coupled with the Original UNIFAC Method and the SRK Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 6836-6845	3.9	7	
1265	Symmetric Nonrandom Two-Liquid Segment Activity Coefficient Model for Electrolytes. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 5522-5529	3.9	12	
1264	Liquid Diquid Equilibria for Systems of 1-Butanol + Water + 2,6-Diaminopyridine and 1-Butanol + Water + 2-Aminopyridine. <i>Journal of Chemical & Data</i> , 2009, 54, 1266-1270	2.8	2	
1263	Isobaric Vapor liquid Equilibria for the Binary Systems Benzene + Methyl Ethanoate, Benzene + Butyl Ethanoate, and Benzene + Methyl Heptanoate at 101.31 kPa Journal of Chemical & Engineering Data, 2009, 54, 1575-1579	2.8	14	
1262	The Solubility of Beclomethasone-17,21-dipropionate in Selected Organic Solvents: Experimental Measurement and Thermodynamic Modeling. 2009 , 13, 1322-1326		4	
1261	Evaluation of Gas Solubility Prediction in Ionic Liquids using COSMOthermX. <i>Journal of Chemical & Engineering Data</i> , 2009 , 54, 2005-2022	2.8	89	
1260	UNIFAC Model for Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 2697-2704	3.9	210	
1259	Kinetic Study of Dowex 50 Wx8-Catalyzed Esterification and Hydrolysis of Benzyl Acetate. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 2519-2532	3.9	32	
1258	An Expression for Ratio of Critical Temperature to Critical Pressure with the Heat Capacity for Low to Medium Molecular Weight Compounds. <i>Journal of Chemical & Description of Chemical & Description (Chemical & Description)</i> , 54, 690-7	იბ ^{.8}	4	
1257	Surface tension of mixed inorganic and dicarboxylic acid aqueous solutions at 298.15 K and their importance for cloud activation predictions. 2009 , 11, 8021-8		36	
1256	Thermodynamic Insights on the Feasibility of Homogeneous Batch Extractive Distillation, 1. Azeotropic Mixtures with a Heavy Entrainer. <i>Industrial & Engineering Chemistry Research</i> , 2009 , 48, 3544-3559	3.9	57	
1255	ThermoData Engine (TDE): software implementation of the dynamic data evaluation concept. 3. Binary mixtures. 2009 , 49, 503-17		39	
1254	Introduction. 2009 , 1-67			
1253	Influence of non-ideality on condensation to aerosol. 2009 , 9, 1325-1337		27	
1252	Amorphous and crystalline aerosol particles interacting with water vapor: conceptual framework and experimental evidence for restructuring, phase transitions and kinetic limitations. 2009 , 9, 9491-95	22	375	
1251	Homogeneous vs. heterogeneous nucleation in water-dicarboxylic acid systems. 2009 , 9, 1873-1881		7	
1250	Composition and properties of atmospheric particles in the eastern Atlantic and impacts on gas phase uptake rates. 2009 , 9, 9299-9314		51	

1249 Separation of Organic Chlorine Compounds through Batch Distillation Process. 2010, 5,

1248	Appendices. 2010 , 141-184	
1247	Computation of liquid-liquid equilibria and phase stabilities: implications for RH-dependent gas/particle partitioning of organic-inorganic aerosols. 2010 , 10, 7795-7820	152
1246	The sensitivity of secondary organic aerosol component partitioning to the predictions of component properties IPart 1: A systematic evaluation of some available estimation techniques. 2010 , 10, 10255-10272	40
1245	Organic particulate matter formation at varying relative humidity using surrogate secondary and primary organic compounds with activity corrections in the condensed phase obtained using a method based on the Wilson equation. 2010 , 10, 5475-5490	23
1244	An Economical Method for Isolation of Dioscin from Dioscorea nipponica Makino by HSCCC Coupled with ELSD, and a Computer-Aided UNIFAC Mathematical Model. 2010 , 71, 15-23	50
1243	Quantitative correlation of physical and chemical properties with chemical structure: utility for prediction. 2010 , 110, 5714-89	372
1242	Multi-scale simulation of the 1,3-butadiene extraction separation process with an ionic liquid additive. 2010 , 12, 1263	32
1241	Making Floryr⊞uggins Practical: Thermodynamics of Polymer-Containing Mixtures. 2010 , 1-66	15
1240	Vapor l iquid equilibria of asymmetrical systems using UNIFAC-NRF group contribution activity coefficient model. <i>Fluid Phase Equilibria</i> , 2010 , 289, 61-71	11
1239	Prediction of aqueous solubilities of solid carboxylic acids with COSMO-RS. <i>Fluid Phase Equilibria</i> , 2010 , 289, 140-147	102
1238	Methane and carbon dioxide solubility in 1,2-propylene glycol at temperatures ranging from 303 to 423K and pressures up to 12MPa. <i>Fluid Phase Equilibria</i> , 2010 , 289, 185-190	8
1237	QSPR analysis of infinite dilution activity coefficients of chlorinated organic compounds in water. Fluid Phase Equilibria, 2010 , 291, 111-116	23
1236	Phase equilibria modeling of biodiesel related mixtures using the GCA-EoS model. <i>Fluid Phase Equilibria</i> , 2010 , 296, 75-81	16
1235	Liquid+liquid equilibria for the quaternary systems of (water+acetic acid+mixed solvent) at 298.2K and atmospheric pressure. <i>Fluid Phase Equilibria</i> , 2010 , 298, 293-297	2
1234	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
1233	Liquid Diquid Equilibrium Constant for Acetic Acid in an Epoxidized Soybean Oil Acetic Acid Water System. 2010 , 87, 591-600	6
1232	Vapour-Liquid Equilibrium with a New Ebulliometer: Ester + Alcohol System at 0.5 MPa. 2010 , 18, 1000-1007	16

1231	Evaluation of a detailed model of secondary organic aerosol formation from pinene against dark ozonolysis experiments. 2010 , 44, 5434-5442	12	
1230	The perception of fragrance mixtures: A comparison of odor intensity models. <i>AICHE Journal</i> , 2010 , 56, NA-NA	7	
1229	Fallstudie zur Vorausberechnung Henryscher Koeffizienten. 2010 , 82, 265-272	2	
1228	A Case Study in the Pre-Calculation of Henry Coefficients. 2010 , 33, 251-257	16	
1227	(Liquid+liquid) equilibrium of (NaClO4+PEG 4000+H2O) ternary system at different temperatures. 2010 , 42, 419-424	12	
1226	Solubility of methane and carbon dioxide in ethylene glycol at pressures up to 14 MPa and temperatures ranging from (303 to 423) K. 2010 , 42, 684-688	32	
1225	Gibbs free energy of transfer of a methylene group on {UCON + (sodium or potassium) phosphate salts} aqueous two-phase systems: Hydrophobicity effects. 2010 , 42, 1063-1069	19	
1224	Measurement and prediction of solubilities of active pharmaceutical ingredients. 2010, 388, 73-81	77	
1223	Vapour l iquid equilibrium for the systems diethyl sulphide+1-butene, +cis-2-butene, +2-methylpropane, +2-methylpropene, +n-butane, +trans-2-butene. <i>Fluid Phase Equilibria</i> , 2010 , 291, 180-187	6	
1222	Boiling point of aqueous d-glucose and d-fructose solutions: Experimental determination and modeling with group-contribution method. <i>Fluid Phase Equilibria</i> , 2010 , 299, 32-41	12	
1221	The solubility and solubility modelling of budesonide in pure and modified subcritical water solutions. 2010 , 55, 37-42	21	
1220	The generalized van der Waals partition function as a basis for excess free energy models. 2010 , 55, 496-502	18	
1219	From van der Waals to VTPR: The systematic improvement of the van der Waals equation of state. 2010 , 55, 438-447	19	
1218	Equations of state: From the ideas of van der Waals to association theories. 2010 , 55, 421-437	41	
1217	Purification process design in the production of styrene monomer. 2010 , 49, 367-375	5	
1216	Comparison of different solubility equations for modeling in cooling crystallization. 2010 , 49, 1284-1297	8	
1215	Liquid II quid equilibrium of the ternary system water+acetic acid+sec-butyl acetate. Fluid Phase Equilibria, 2010, 293, 73-78	11	
1214	Test of athermal terms of activity coefficient models by Monte Carlo simulation with hard-core models. <i>Fluid Phase Equilibria</i> , 2010 , 297, 221-226	1	

1213	Zur Korrelation von Grenzaktivit Eskoeffizienten und Aktivit Eskoeffizienten in endlichen Konzentrationsbereichen unter Anwendung moderner Inkrementen- und mathematischer Verfahren. 2010 , 18, 81-88		2
1212	Normierung und Berechnung von Ionenaktivit Eskoeffizienten in elekrolythaltigen gemischten L Bungsmitteln aus Messungen des Fl Sigkeits-Dampf-Gleichgewichts. 2010 , 19, 201-205		
1211	Modeling of Esterification in a Batch Reactor Coupled with Pervaporation for Production of n-Butyl Acetate. 2010 , 31, 999-1005		11
121 0	Benzene inhalation by parts washers: new estimates based on measures of occupational exposure to solvent coaromatics. 2010 , 30, 1249-67		9
1209	VLE Data of Methyl Acetate + Methanol at 1.0, 3.0 and 7.0 Bar with a New Ebulliometer. 2010 , 43, 650-656		18
1208	Solvent design for a Menschutkin reaction by using CAMD and DFT calculations. 2010 , 28, 1291-1296		2
1207	Diffusion of oligomers in latex systems IA route to low volatile organic compound (VOC) coatings. 2010 , 88, 500-513		4
1206	Effect of Aerosol Generation Method on Measured Saturation Pressure and Enthalpy of Vaporization for Dicarboxylic Acid Aerosols. 2010 , 44, 302-307		13
1205	Theoretical versus observed gas-particle partitioning of carbonyl emissions from motor vehicles. 2010 , 60, 1237-44		2
1204	Empirical and theoretical models of equilibrium and non-equilibrium transition temperatures of supplemented phase diagrams in aqueous systems (IUPAC Technical Report). 2010 , 82, 1065-1097		43
1203	Extension of GMA Equation of State to Long-Chain Alkanes Using Group Contribution Method. Industrial & Company Company Contribution Method. 3-9		10
1202	Chapter 13:Equations of State in Chemical Reacting Systems. 2010 , 433-459		1
1201	Quality Assessment Algorithm for Vaporlliquid Equilibrium Data. <i>Journal of Chemical & amp;</i> Engineering Data, 2010 , 55, 3631-3640	í	102
1200	Research Progress on Flash Point Prediction. <i>Journal of Chemical & Engineering Data</i> , 2010 , 55, 2943 <u>2</u> 8	950	56
1199	Using an Adaptive Parameter Method for Process Simulation of Nonideal Systems. <i>Industrial & amp; Engineering Chemistry Research</i> , 2010 , 49, 4923-4932	1	10
1198	Surface Tensions of the Ternary Mixtures Containing an Isomeric Butanol +n-Hexane + 1-Chlorobutane at 298.15 K. <i>Journal of Chemical & Data</i> , 2010 , 55, 3532-3537		8
1197	Gas-particle partitioning of alcohol vapors on organic aerosols. 2010 , 44, 257-62		6
1196	Vapor l liquid Equilibrium for Binary Systems of Cyclohexane + Cyclohexanone and + Cyclohexanol at Temperatures from (414.0 to 433.7) K. <i>Journal of Chemical & Data, 2010, 55, 3418-342</i> 8		7

1195	Solubility and Miscibility for the Mixture of (Ethyl Fluoride + Polyol Ester Oil). <i>Journal of Chemical & Engineering Data</i> , 2010 , 55, 3200-3207	2.8	21	
1194	Solubility and Micronization of Griseofulvin in Subcritical Water. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 3403-3410	3.9	37	
1193	Isothermal Binary Vapor liquid Equilibrium for 2-Methylpropane and n-Butane with 1,2-Ethanedithiol and 2-Methyl-2-propanethiol. <i>Journal of Chemical & Description of Chemical & Description</i> 1,2-Ethanedithiol and 2-Methyl-2-propanethiol. <i>Journal of Chemical & Description</i> 2010, 55, 291-296	2.8	5	
1192	Prediction of Homogeneous Azeotropes by the UNIFAC Method for Binary Refrigerant Mixtures. Journal of Chemical & Data, 2010, 55, 52-57	2.8	3	
1191	Observation of the suppression of water uptake by marine particles. 2010 , 98, 219-228		12	
1190	Prediction of environmental parameters of polycyclic aromatic hydrocarbons with COSMO-RS. 2010 , 79, 821-9		19	
1189	Solubility, Solubility Modeling, and Precipitation of Naproxen from Subcritical Water Solutions. <i>Industrial & Discrete Engineering Chemistry Research</i> , 2010 , 49, 9385-9393	3.9	21	
1188	UNIFAC Group Interaction Prediction for Ionic Liquid-Thiophene Based Systems Using Genetic Algorithm. 2010 , 195-204		3	
1187	Modeling of Highly Nonideal Systems: 2. Prediction of High Pressure Phase Equilibria with the Group Contribution NRTL-PR EoS. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 7589-7596	3.9	12	
1186	Solubility Model of Solid Solute in Supercritical Fluid Solvent Based on UNIFAC. <i>Industrial & Engineering Chemistry Research</i> , 2010 , 49, 5952-5957	3.9	7	
1185	Simultaneous Prediction of Densities and Vaporliquid Equilibria of Mixtures Containing an Isomeric Chlorobutane and Methyl tert-Butyl Ether Using the VTPR Model. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 14193-14202	3.9	4	
1184	Liquid Liquid Equilibrium Calculation for Ternary Aqueous Mixtures of Ethanol and Acetic Acid with 2-Ethyl-1-hexanol Using the GMDH-Type Neural Network. <i>Industrial & Description of the Mixed Research</i> , 2011 , 50, 10158-10167	3.9	2	
1183	Purification and Recovery of Curcuminoids from Curcuma longa Extract by Reactive Sorption Using Polymeric Adsorbent Carrying Tertiary Amine Functional Group. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 7452-7461	3.9	7	
1182	Liquidliquid and Vaporliquidliquid Equilibrium of the 4-Methyl-2-pentanone + 2-Butanol + Water System. <i>Journal of Chemical & Engineering Data</i> , 2011 , 56, 1925-1932	2.8	13	
1181	Modeling Phase Equilibria Relevant to Biodiesel Production: A Comparison of gE Models, Cubic EoS, EoSBE and Association EoS. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 2348-2358	3.9	31	
1180	Liquidliquid and Vaporliquidliquid Equilibrium of the 2-Butanone + 2-Butanol + Water System. Journal of Chemical & Data, 2011, 56, 1755-1761	2.8	11	
1179	Experimental and Predicted Kinematic Viscosities for Alkane + Chloroalkane Mixtures. <i>Journal of Chemical & Ch</i>	2.8	23	
1178	Evaluation of Group-Contribution Methods To Predict VLE and Odor Intensity of Fragrances. Industrial & Engineering Chemistry Research, 2011, 50, 9390-9402	3.9	17	

1177	ThermoData Engine (TDE): software implementation of the dynamic data evaluation concept. 5. Experiment planning and product design. 2011 , 51, 181-94		25
1176	Analytical modeling of degradation product partitioning kinetics in source zones containing entrapped DNAPL. 2011 , 47,		6
1175	Solubility Calculation of Active Pharmaceutical Ingredients in Alkanes, Alcohols, Water and their Mixtures Using Various Activity Coefficient Models. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 1757-1769	3.9	40
1174	Improvement of the dissolution rate of poorly soluble drugs by solid crystal suspensions. 2011 , 8, 727-3	5	47
1173	My contribution to broadening the base of chemical engineering. 2011 , 2, 1-7		7
1172	Solidliquid Equilibria in Fatty Acid/Triglycerol Systems. <i>Journal of Chemical & Data</i> , 2011 , 56, 1613-1616	2.8	18
1171	Application of the Unified Functional Activity Coefficient (UNIFAC) and Analytical Solution of Groups (ASOG) for the Calculation of Mutual Solubilities in Water Systems of Alkanes, Arenes, and Alkanols. <i>Journal of Chemical & Engineering Data</i> , 2011 , 56, 4853-4861	2.8	10
1170	Molecular Thermodynamic Modeling and Design of Microencapsulation Systems for Drug Delivery. Journal of Chemical & Engineering Data, 2011, 56, 1229-1237	2.8	5
1169	Solubility of Polymers. 2011 ,		3
1168	Entropies of Condensed Phases and Complex Systems. 2011 ,		12
1167	Determination of Chlorobenzene Solubilities in Subcritical Water in a Fused Silica Capillary Reactor from 173 to 267 °C. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 11724-11727	3.9	17
1166	Prediction of Liquid Liquid Equilibria for Biofuel Applications by Quantum Chemical Calculations Using the Cosmo-SAC Method. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 13066-13075	3.9	25
1165	Thermodynamic Model for the Prediction of Equilibrium Conditions of Clathrate Hydrates of Methane + Water-Soluble or -Insoluble Hydrate Former. <i>Industrial & Engineering Chemistry Research</i> , 2011 , 50, 9437-9450	3.9	28
1164	An Ideal Absorbed Solution Theory (IAST) Study of Adsorption Equilibria of Binary Mixtures of Methane and Ethane on a Templated Carbon. <i>Journal of Chemical & Engineering Data</i> , 2011 , 56, 120) 3 :821	2 ³⁹
1163	Solubilities of Betulinic Acid in Thirteen Organic Solvents at Different Temperatures. <i>Journal of Chemical & Different Temperatures</i> . <i>Journal of Chemical & Different Temperatures</i> . <i>Journal of Chemical & Different Temperatures</i> .	2.8	51
1162	Modeling the Influence of Molecular Interactions on the Vaporization of Multi-component Fuel Sprays. 2011 ,		10
1161	Relating hygroscopicity and composition of organic aerosol particulate matter. 2011 , 11, 1155-1165		268
1160	The sensitivity of secondary organic aerosol (SOA) component partitioning to the predictions of component properties IPart 3: Investigation of condensed compounds generated by a near-explicit model of VOC oxidation. 2011 , 11, 13145-13159		19

1159	A two-dimensional volatility basis set: 1. organic-aerosol mixing thermodynamics. 2011 , 11, 3303-3318	421
1158	Temperature-induced volatility of molecular markers in ambient airborne particulate matter. 2011 , 11, 67-76	16
1157	The sensitivity of Secondary Organic Aerosol component partitioning to the predictions of component properties (Part 2: Determination of particle hygroscopicity and its dependence on "apparent" volatility. 2011 , 11, 7767-7779	25
1156	Estimating fusion properties for functionalised acids. 2011 , 11, 8385-8394	8
1155	Modeling secondary organic aerosol formation from isoprene oxidation under dry and humid conditions. 2011 , 11, 893-909	42
1154	New and extended parameterization of the thermodynamic model AIOMFAC: calculation of activity coefficients for organic-inorganic mixtures containing carboxyl, hydroxyl, carbonyl, ether, ester, alkenyl, alkyl, and aromatic functional groups. 2011 , 11, 9155-9206	240
1153	Group Contribution Methodologies for the Prediction of Thermodynamic Properties and Phase Behavior in Mixtures. 2011 , 135-172	3
1152	Measuring and predicting head space pressure during retorting of thermally processed foods. 2011 , 76, E298-308	4
1151	Supercritical hydrothermal synthesis of metallic cobalt nanoparticles and its thermodynamic analysis. 2011 , 60, 113-120	40
1150	Application of the modified linear isotherm regularity equation of state to long chain amines and esters. 2011 , 526, 35-45	
1149	Kinetic limitations on tracer partitioning in ganglia dominated source zones. 2011 , 126, 195-207	4
1148	Solid-Liquid Equilibria of D-Glucose, D-Fructose and Sucrose in the Mixture of Ethanol and Water from 273.2 K to 293.2 K. 2011 , 19, 217-222	28
1147	Isothermal vapour[Iquid equilibria and excess enthalpies for the binary mixtures containing an isomeric chlorobutane and diisopropyl ether. <i>Fluid Phase Equilibria</i> , 2011 , 308, 8-14	6
1146	An evaluation of thermodynamic models for the prediction of drug and drug-like molecule solubility in organic solvents. <i>Fluid Phase Equilibria</i> , 2011 , 309, 36-52	56
1145	A new method for evaluation of UNIFAC interaction parameters. <i>Fluid Phase Equilibria</i> , 2011 , 309, 68-75 2.5	25
1144	Solid Ilquid equilibrium data for the binary system methacrylic acid+methanol in the high methacrylic acid concentration range. <i>Fluid Phase Equilibria</i> , 2011 , 312, 14-19	4
1143	Atmospheric amines [Part II. Thermodynamic properties and gas/particle partitioning. 2011, 45, 561-577	187
1142	Ionic liquids: predictions of physicochemical properties with experimental and/or DFT-calculated LFER parameters to understand molecular interactions in solution. 2011 , 115, 6040-50	49

1141 A priori calculations of adsorption equilibria in ternary systems. **2011**, 47, 562-565

1140	Predicting Infinite Dilution Activity Coefficients of Chlorinated Organic Compounds in Aqueous Solution Based on Three-Dimensional WHIM and GETAWAY Descriptors. 2011 , 40, 118-130		5
1139	Thermodynamic study of non-solvent/dimethyl sulfoxide/polyacrylonitrile ternary systems: effects of the non-solvent species. 2011 , 67, 1073-1089		20
1138	Impact of sorption phenomena on multiphase conveying processes. 2011 , 47, 921-931		1
1137	Thermodynamics of mixtures containing oxaalkanes. 5. Ether+benzene, or +toluene systems. <i>Fluid Phase Equilibria</i> , 2011 , 301, 145-155	2.5	18
1136	Liquid II quid equilibrium for the ternary systems of water+acetyl acetone+propyl acetate at several temperatures. <i>Fluid Phase Equilibria</i> , 2011 , 304, 7-11	2.5	12
1135	Phase equilibria of (waterdarboxylic aciddiethyl maleate) ternary liquid systems at 298.15K. <i>Fluid Phase Equilibria</i> , 2011 , 303, 168-173	2.5	26
1134	The solid[Iquid equilibrium of the binary system H2ODMSO and the influence of a salt (NaCl, KCl) on the thermodynamic behavior: Correlations using a revised LIQUAC model. <i>Fluid Phase Equilibria</i> , 2011 , 304, 12-20	2.5	11
1133	Extension of polar GC-SAFT to systems containing some oxygenated compounds: Application to ethers, aldehydes and ketones. <i>Fluid Phase Equilibria</i> , 2011 , 307, 142-159	2.5	47
1132	(Liquid + liquid) equilibrium of (NaNO3 + PEG 4000 + H2O) ternary system at different temperatures. 2011 , 43, 1573-1578		28
1131	A generalized reference state at constant volume for the prediction of phase equilibria from low pressure model parameters: Application to size-asymmetric systems and to the WongBandler mixing rule. 2011 , 66, 4148-4156		7
1130	Design of formulated products: A systematic methodology. <i>AICHE Journal</i> , 2011 , 57, 2431-2449	3.6	103
1129	Process Analysis and Multi-Objective Optimization of Ionic Liquid-Containing Acetonitrile Process to Produce 1,3-Butadiene. 2011 , 34, 927-936		12
1128	Inverse exergo-🏿 Rologisch-🗘 Ronomische Prozessanalyse von Abgasbehandlungsprozessen. 2011 , 83, 427-442		2
1127	Equation of state for square-well chain molecules with variable range, extension to associating fluids. <i>Fluid Phase Equilibria</i> , 2011 , 302, 139-152	2.5	5
1126	Thermodynamic modeling of phase equilibria in biorefineries. <i>Fluid Phase Equilibria</i> , 2011 , 302, 1-9	2.5	27
1125	On the compatibility between vapor pressure data and the critical constants: Use of the van der Waals family of cubic equations of state to study the cases of 2-methoxyethanol and 2-ethoxyethanol. <i>Fluid Phase Equilibria</i> , 2011 , 303, 201-204	2.5	3
1124	Simultaneous prediction of vapour即quid and liquid即quid equilibria (VLE and LLE) of aqueous mixtures with the SAFT-胸roup contribution approach. <i>Fluid Phase Equilibria</i> , 2011 , 306, 82-96	2.5	49

1123	A review of subcritical water as a solvent and its utilisation for the processing of hydrophobic organic compounds. 2011 , 172, 1-17		225
1122	Integrated solvent and process design using a SAFT-VR thermodynamic description: High-pressure separation of carbon dioxide and methane. 2011 , 35, 474-491		73
1121	Co-evaporative multi-component fuel design for in-cylinder PLIF measurement and application in gasoline direct injection research. 2011 , 88, 2617-2627		27
1120	Prediction of miscible mixtures flash-point from UNIFAC group contribution methods. <i>Fluid Phase Equilibria</i> , 2011 , 300, 70-82	2.5	57
1119	Application of GC-PPC-SAFT EoS to amine mixtures with a predictive approach. <i>Fluid Phase Equilibria</i> , 2011 , 303, 15-30	2.5	26
1118	Solid l Iquid equilibrium using the SAFT-VR equation of state: Solubility of naphthalene and acetic acid in binary mixtures and calculation of phase diagrams. <i>Fluid Phase Equilibria</i> , 2011 , 306, 137-147	2.5	8
1117	pePC-SAFT: Modeling of polyelectrolyte systems 2. Aqueous two-phase systems. <i>Fluid Phase Equilibria</i> , 2011 , 306, 67-75	2.5	10
1116	Calculation of permeabilities and numerical simulation of separations for volatile organic compound vapor through triethylene glycol derivative liquid membranes. 2011 , 369, 448-454		2
1115	Hazard assessment of edible oil refining: Formation of flammable mixtures in storage tanks. 2011 , 105, 105-111		9
1114	Solubility of fragrance raw materials in water: Experimental study, correlations, and Mod. UNIFAC (Do) predictions. 2011 , 43, 28-33		2
1113	Polymer Thermodynamics. 2011,		4
1112	Advanced REACH Tool: development and application of the substance emission potential modifying factor. 2011 , 55, 980-8		17
1111	Simultaneous prediction of phase behaviour and second derivative properties with a group contribution approach (SAFT-∰Mie). 2011 , 1593-1597		
1110	A Semi-Empirical Model for Condensation Heat Transfer Coefficient of Mixed Ethanol-Water Vapors. 2011 , 133,		9
1109	Partial Derivative Fitted Taylor Expansion: an efficient method for calculating gas/liquid equilibria in atmospheric aerosol particles Part 2: Organic compounds. 2011 ,		1
1108	Partial Derivative Fitted Taylor Expansion: an efficient method for calculating gas/liquid equilibria in atmospheric aerosol particles Part 2: Organic compounds. 2012 , 5, 1-13		13
1107	Flash-Point Prediction of Binary Partially Miscible Aqueous-Organic Mixtures from UNIFAC Group Contribution Methods. 2012 , 560-561, 1178-1183		4
1106	Modeling of solubility of CO2 in 1-butylpyridinium bis(trifluoromethylsulfonyl)imide ionic liquid using UNIFAC. 2012 ,		5

1105	Volatility and aging of atmospheric organic aerosol. 2014 , 339, 97-143		56
1104	Organic Solvents for Separating Ethyl Acetate-Ethanol by Extractive Distillation. 2012 , 550-553, 699-703		
1103	New representation of water activity based on a single solute specific constant to parameterize the hygroscopic growth of aerosols in atmospheric models. 2012 , 12, 5429-5446		10
1102	Ethanol and Distillate Blends: A Thermodynamic Approach to Miscibility Issues: Part 3 [] Generalization to Other Alcohols (Methanol, Isopropanol and 1-Butanol). 2012 ,		
1101	Modeling the gas-particle partitioning of secondary organic aerosol: the importance of liquid-liquid phase separation. 2012 , 12, 3857-3882		179
1100	Parameterising secondary organic aerosol from pinene using a detailed oxidation and aerosol formation model. 2012 , 12, 5343-5366		9
1099	Tight coupling of particle size, number and composition in atmospheric cloud droplet activation. 2012 , 12, 3253-3260		63
1098	Control of Liquid Membrane Separation Process. 2012 , 85-100		
1097	A Thermodynamic Model for Vaporliquid Equilibrium Data for the Two Binary Systems. 2012 , 11-16		
1096	Thirty Years with EoS/GEModelsWhat Have We Learned?. <i>Industrial & Description of the Market </i>	.9	54
1095	Vaporliquid Equilibria Measurements of Bitter Orange Aroma Compounds Highly Diluted in Boiling Hydro-Alcoholic Solutions at 101.3 kPa. <i>Journal of Chemical & Data</i> , 2012, 57, 3344-3356	8	10
1094	Rapid Crystallization Process Development Strategy from Lab to Industrial Scale with PAT Tools in Skid Configuration. 2012 , 16, 769-780		14
1093	Application of the Conduct-like Screening Models for Real Solvent and Segment Activity Coefficient for the Predictions of Partition Coefficients and Vaporliquid and Liquidliquid Equilibria of Bio-oil-Related Mixtures. 2012 , 26, 3756-3768		9
1092	Working Pair Selection of Compression and Absorption Hybrid Cycles through Predicting the Activity Coefficients of Hydrofluorocarbon + Ionic Liquid Systems by the UNIFAC Model. <i>Industrial & amp; Engineering Chemistry Research</i> , 2012 , 51, 4741-4747	.9	48
1091	Solubility of l-Phenylalanine Anhydrous and Monohydrate Forms: Experimental Measurements and Predictions. <i>Journal of Chemical & Data</i> , 2012 , 57, 1492-1498	8	33
1090	Non-equilibrium compressible lattice theories accounting for hydrogen bonding interactions: Modelling water sorption thermodynamics in fluorinated polyimides. <i>Fluid Phase Equilibria</i> , 2012 , 234, 166-188	5	25
1089	Vapourliquid and vapourliquidliquid equilibrium modeling for binary, ternary, and quaternary systems of solvents. <i>Fluid Phase Equilibria</i> , 2012 , 333, 97-105	5	7
1088	Phase equilibria of toluene/heptane with tetrabutylphosphonium bromide based deep eutectic solvents for the potential use in the separation of aromatics from naphtha. <i>Fluid Phase Equilibria</i> , 2012, 333, 47-54	5	76

1087	Solubility of organic solvents in 1,4-cis-polybutadiene. Fluid Phase Equilibria, 2012, 334, 10-14	2.5	4
1086	Thermodynamic model for prediction of phase equilibria of clathrate hydrates of hydrogen with different alkanes, alkenes, alkynes, cycloalkanes or cycloalkene. <i>Fluid Phase Equilibria</i> , 2012 , 336, 71-78	2.5	21
1085	Study of Minimum Flash-point Behavior for Ternary Mixtures of Flammable Solvents. 2012 , 45, 507-511		4
1084	Investigation of the relationships between the thermodynamic phase behavior and gelation behavior of a series of tripodal trisamide compounds. 2012 , 8, 6483		27
1083	Measurements of thermodynamic and optical properties of selected aqueous organic and organic-inorganic mixtures of atmospheric relevance. 2012 , 116, 9954-68		50
1082	COSMOquick: A Novel Interface for Fast Profile Composition and Its Application to COSMO-RS Solvent Screening Using Multiple Reference Solvents. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 14303-14308	3.9	34
1081	Product Separation after Chemical Interesterification of Vegetable Oils with Methyl Acetate. Part I: Vaporliquid Equilibrium. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 8087-8094	3.9	8
1080	Thermodynamic Characterization of Undefined Petroleum Fractions using Group Contribution Methods. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 14188-14198	3.9	19
1079	Esterification of Acrylic Acid and n-Butanol in a Pilot-Scale Reactive Distillation Column E xperimental Investigation, Model Validation, and Process Analysis. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 16444-16456	3.9	31
1078	Product Separation after Chemical Interesterification of Vegetable Oils with Methyl Acetate. Part II: Liquid Liquid Equilibrium. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 10201-10206	3.9	9
1077	ThermoData Engine (TDE) software implementation of the dynamic data evaluation concept. 7. Ternary mixtures. 2012 , 52, 260-76		26
1076	Deliquescence and efflorescence behavior of ternary inorganic/organic/water aerosol particles. 2012 , 116, 6199-210		29
1075	Optimal Solvent Screening for the Crystallization of Pharmaceutical Compounds from Multisolvent Systems. <i>Industrial & Discourt Amp; Engineering Chemistry Research</i> , 2012 , 51, 13792-13802	3.9	21
1074	Solubilities of Protocatechuic Aldehyde, Caffeic Acid, d-Galactose, and d-Raffinose Pentahydrate in Ethanol Water Solutions. <i>Journal of Chemical & Ethanol Water Solutions</i> 2012, 57, 2018-2022	2.8	22
1073	Adsorption and Kinetic Parameters for Synthesis of Methyl Nonanoate over Heterogeneous Catalysts. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 14367-14375	3.9	23
1072	Solubilities of 3-Methoxy-N-phenylaniline and 3-(Methylthio)-N-phenylaniline in Five Organic Solvents (285 K to 333.75 K). <i>Journal of Chemical & Data, Engineering Data, 2012</i> , 57, 1581-1585	2.8	14
1071	Estimating Octanol Water Partition Coefficients for Selected Nanoscale Building Blocks Using the COSMO-SAC Segment Contribution Method. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 4556-4566	3.9	4
1070	Thermodynamical methods for the optimization of lipase-catalyzed reactions. 2012 , 861, 383-400		5

1069	Isothermal Vaporlliquid Equilibrium Data for the Propan-1-ol + Dodecane System at (323.0, 343.4, 353.2, 363.1, and 369.2) K. <i>Journal of Chemical & Engineering Data</i> , 2012 , 57, 862-868	2.8	5
1068	LiquidIquid equilibrium of 1-propanol, 2-propanol, 2-methyl-2-propanol or 2-butanol + sodium sulfite + water aqueous two phase systems. <i>Fluid Phase Equilibria</i> , 2012 , 329, 42-54	2.5	21
1067	Thermodynamic properties and vaporliquid equilibria of associating fluids, PengRobinson equation of state coupled with shield-sticky model. <i>Fluid Phase Equilibria</i> , 2012 , 330, 1-11	2.5	2
1066	Ternary liquid[Iquid phase equilibria of (waterflarboxylic acidfl-undecanol) systems at 298.15K. Fluid Phase Equilibria, 2012 , 331, 26-32	2.5	24
1065	Development of an EOS based on lattice cluster theory for pure components. <i>Fluid Phase Equilibria</i> , 2012 , 331, 58-79	2.5	18
1064	Introduction Of The Group Contribution Concept Into The Nrtl Model. 2012 , 18, 1182-1188		4
1063	Extension of the UNIFAC Model for Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 12135-12144	3.9	107
1062	Characterization of the Solvent Properties of Glycerol Using Inverse Gas Chromatography and Solubility Parameters. 2012 , 89, 1585-1597		7
1061	Isobaric Vaporlliquid Equilibrium of the Mixture of Methyl Palmitate and Methyl Stearate at 0.1 kPa, 1 kPa, 5 kPa, and 10 kPa. <i>Journal of Chemical & Engineering Data</i> , 2012 , 57, 2632-2639	2.8	16
1060	Liquid Liquid Equilibria in Ternary Mixtures of Methyl Oleate + Ethanol + Glycerol at Atmospheric Pressure. <i>Industrial & amp; Engineering Chemistry Research</i> , 2012 , 51, 9642-9651	3.9	10
1059	Comparison of the a Priori COSMO-RS Models and Group Contribution Methods: Original UNIFAC, Modified UNIFAC(Do), and Modified UNIFAC(Do) Consortium. <i>Industrial & amp; Engineering Chemistry Research</i> , 2012 , 51, 11809-11817	3.9	31
1058	The Importance of Acetonitrile in the Pharmaceutical Industry and Opportunities for its Recovery from Waste. 2012 , 16, 612-624		76
1057	Top-cited Articles in Chemical Engineering in Science Citation Index Expanded: A Bibliometric Analysis. 2012 , 20, 478-488		108
1056	A hydrophilic/hydrophobic organic (H2O) aerosol model: Development, evaluation and sensitivity analysis. 2012 , 117, n/a-n/a		67
1055	Liquid Liquid Equilibrium of Some Aliphatic Alcohols + Disodium Tartrate + Water Aqueous Two-Phase Systems at 298.15 K. <i>Journal of Chemical & Data</i> , 2012, 57, 2336-2342	2.8	10
1054	Distillation and Gas Absorption. 2012 , 399-486		
1053	Solubility Prediction of Pharmaceutical and Chemical Compounds in Pure and Mixed Solvents Using Predictive Models. <i>Industrial & Engineering Chemistry Research</i> , 2012 , 51, 464-473	3.9	38
1052	Profit maximization of the normal hexane recovery process through a thermal integration method. 2012 , 29, 1239-1245		

1051	Measurement and correlation of the isothermal vapor-liquid equilibrium data for carbon dioxide and dimethyl ether system. 2012 , 29, 1418-1425		6
1050	Lipases and Phospholipases. 2012 ,		12
1049	Properties. 2012 , 401-421		4
1048	Solubility of Xylose, Mannose, Maltose Monohydrate, and Trehalose Dihydrate in Ethanol Water Solutions. <i>Journal of Chemical & Data</i> , 2012, 57, 3264-3269		29
1047	Thermodynamics in Food Process Design. 2012 , 74-112		
1046	Methodologies for Fuel Cell Process Engineering. 2012 , 597-644		4
1045	On The Incompatibility of Dextran and Pullulan in Aqueous Solutions and Its Modeling. 2012 , 213, 1206-121	5	3
1044	Thermodynamics and transport properties of citral. <i>AICHE Journal</i> , 2012 , 58, 2557-2562 3.6		8
1043	Hydration of Saccharides: Estimation of Reaction Properties and Equilibrium Conversion. 2012 , 35, 735-742		0
1042	Characterization of Feed Properties for Conceptual Process Design Involving Complex Mixtures. 2012 , 84, n/a-n/a		2
1041	Estimating the flammability of vapours above refinery wastewater laden with hydrocarbon mixtures. 2012 , 51, 61-67		8
1040	Predictions of high pressure phase equilibria of CO2-containing mixtures with the NRCOSMO model. <i>Fluid Phase Equilibria</i> , 2012 , 313, 203-210		1
1039	Thermodynamic modeling of pressureDemperature phase diagrams of binary clathrate hydrates of methane, carbon dioxide or nitrogen + tetrahydrofuran, 1,4-dioxane or acetone. <i>Fluid Phase</i> 2.5 <i>Equilibria</i> , 2012 , 320, 32-37		35
1038	Measurement of VLE data of carbon dioxide+dimethyl carbonate system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol. <i>Fluid Phase Equilibria</i> , 2012 , 318, 77-82		18
1037	Calculation of drug-like molecules solubility using predictive activity coefficient models. <i>Fluid Phase Equilibria</i> , 2012 , 322-323, 48-55		15
1036	Mathematical model of liquid[Iquid equilibrium for a ternary system using the GMDH-type neural network and genetic algorithm. 2012 , 36, 4096-4105		41
1035	Computation of liquid[Iquid equilibrium of organic-ionic liquid systems using NRTL, UNIQUAC and NRTL-NRF models. 2012 , 171, 43-49		34
1034	Thermodynamically based solvent design for enzymatic saccharide acylation with hydroxycinnamic acids in non-conventional media. 2012 , 29, 255-70		16

1033	Effect of mixing rule boundary conditions on high pressure (liquid+liquid) equilibrium prediction. 2012 , 47, 33-41		7
1032	Experimental and predicted properties of the binary mixtures containing an isomeric chlorobutane and butyl ethyl ether. 2012 , 51, 150-158		6
1031	Partial solvation parameters and LSER molecular descriptors. 2012 , 51, 172-189		25
1030	Extraction of aromatics from petroleum naphtha reformate by solvent: UNIFAC modelling and optimization of solvent consumption. 2012 , 53, 30-35		1
1029	Determination of LFER descriptors of 30 cations of ionic liquidsprogress in understanding their molecular interaction potentials. 2012 , 13, 780-7		11
1028	Calculation of the solubility of liquid solutes in glassy polymers. AICHE Journal, 2012, 58, 292-301	3.6	31
1027	Solubility and diffusivity of cyclohexane in high density polyethylene. 2012, 124, 4315-4321		9
1026	Kinetic study of the esterification of acetic acid and n-amyl alcohol catalyzed by H3PW6Mo6O40 immobilized on silylated palygorskite. 2013 , 110, 163-175		2
1025	Physical Properties and Thermodynamic Models. 2013 , 3, 57-89		1
1024	Development of a Group Contribution Method Based on UNIFAC Groups for the Estimation of Vapor Pressures of Pure Hydrocarbon Compounds. 2013 , 36, 483-491		28
1023	Isobaric vaporllquid equilibria of the binary system acetone + acetone oxime methyl ether at 101.3 kPa. <i>Fluid Phase Equilibria</i> , 2013 , 342, 42-46	2.5	6
1022	Design of Perfumes. 2013, 15-60		1
1021	Separation of Azeotropic Mixtures. 2013 , 179-213		1
1020	LLE experimental data, thermodynamic modeling and sensitivity analysis in the ethyl biodiesel from macauba pulp oil settling step. 2013 , 131, 468-75		30
1019	Quantitative NMR spectroscopy of binary liquid mixtures (aldehyde+alcohol). Part II: (Propanal or butanal or heptanal)+(methanol or ethanol or 1-propanol). 2013 , 65, 233-246		2
1018	Molecular mechanism of deactivation of C. antarctica lipase B by methanol. 2013 , 168, 462-9		38
1017	Liquid II quid equilibrium of fatty systems: A new approach for adjusting UNIFAC interaction parameters. <i>Fluid Phase Equilibria</i> , 2013 , 360, 379-391	2.5	26
1016	Flash points of partially miscible aqueousBrganic mixtures predicted by UNIFAC group contribution methods. <i>Fluid Phase Equilibria</i> , 2013 , 345, 45-59	2.5	16

1015	The role of activity coefficients in bioreaction equilibria: thermodynamics of methyl ferulate hydrolysis. 2013 , 173-174, 21-30		27	
1014	Phase equilibrium of the CO2/glycerol system: Experimental data by in situ FT-IR spectroscopy and thermodynamic modeling. 2013 , 73, 97-107		36	
1013	Determination and Correlation of Solubility Data and Dissolution Thermodynamic Data of l-Lactide in Different Pure Solvents. <i>Journal of Chemical & Data, Engineering Data, 2013, 58, 143-150</i>	2.8	15	
1012	Suitability prediction and affinity regularity assessment of H2O+imidazolium ionic liquid working pairs of absorption cycle by excess property criteria and UNIFAC model. <i>Fluid Phase Equilibria</i> , 2013 , 348, 1-8	2.5	26	
1011	Toluene Sorption in Poly(styrene) and Poly(vinyl acetate) near the Glass Transition. <i>Industrial & Engineering Chemistry Research</i> , 2013 , 52, 8917-8927	3.9	11	
1010	Advances in Food Process Engineering Research and Applications. 2013,		5	
1009	Non-ideality and Solubility Modeling of Amino Acids and Peptides in Aqueous Solutions: New Physical and Chemical Approach. <i>Industrial & Engineering Chemistry Research</i> , 2013 , 52, 16044-160.	5 <i>6</i> ∙9	14	
1008	A Knowledge Base for The Recovery of Natural Phenols with Different Solvents. 2013 , 16, 382-396		182	
1007	ThermoData Engine (TDE): software implementation of the dynamic data evaluation concept. 9. Extensible thermodynamic constraints for pure compounds and new model developments. 2013 , 53, 3418-30		23	
1006	Fluid-mineral equilibria and thermodynamic mixing properties of fluid systems. 2013 , 21, 539-549		15	
1005	Numerical simulation of evaporation and drying of a bi-component droplet. 2013, 66, 404-411		30	
1004	Solute recovery from ionic liquids: A conceptual design study for recovery of styrene monomer from [4-mebupy][BF4]. 2013 , 70, 148-161		18	
1003	Thermodynamics of ketone+amine mixtures. Part IX. Excess molar enthalpies at 298.15K for dipropylamine, or dibutylamine+2-alkanone systems and modeling of linear or aromatic amine+2-alkanone mixtures in terms of DISQUAC and ERAS. <i>Fluid Phase Equilibria</i> , 2013 , 343, 1-12	2.5	12	
1002	Measurement and correlation of vaporliquid equilibria for alkane+alkanol and alkane+alkanediol systems with group contribution COSMOSPACE model. <i>Fluid Phase Equilibria</i> , 2013 , 357, 24-29	2.5	1	
1001	Computer-aided design of tailor-made ionic liquids. AICHE Journal, 2013, 59, 4627-4640	3.6	78	
1000	Phase equilibrium of (water+formic or acetic acid+ethyl heptanoate) ternary liquid systems at different temperatures. <i>Fluid Phase Equilibria</i> , 2013 , 356, 71-77	2.5	12	
999	Application of the cubic-plus-association (CPA) equation of state to model the fluid phase behaviour of binary mixtures of water and tetrahydrofuran. <i>Fluid Phase Equilibria</i> , 2013 , 356, 209-222	2.5	11	
998	Synthesis of dimethyl carbonate and propylene glycol in a pilot-scale reactive distillation column: Experimental investigation, modeling and process analysis. 2013 , 234, 448-463		41	

997	Salting-out effect of sodium, potassium, carbonate, sulfite, tartrate and thiosulfate ions on aqueous mixtures of acetonitrile or 1-methyl-2-pyrrolidone: A liquid I quid equilibrium study. Fluid Phase Equilibria, 2013, 360, 357-366	.5	18
996	Computer-aided molecular design of solvents for accelerated reaction kinetics. 2013 , 5, 952-7		117
995	Thermodynamics of ketone+amine mixtures. Part X. Excess molar enthalpies at 298.15K for N,N,N-triethylamine+2-alkanone systems. Characterization of tertiary amine+2-alkanone, and of amino-ketone+n-alkane mixtures in terms of DISQUAC. <i>Fluid Phase Equilibria</i> , 2013 , 356, 117-125	.5	13
994	Synthesis of dimethyl carbonate and propylene glycol by transesterification of propylene carbonate with methanol: Catalyst screening, chemical equilibrium and reaction kinetics. 2013 , 104, 347-3	360	38
993	Application of deep eutectic solvents for the separation of aliphatics and aromatics. 2013,		2
992	New Approach for Absorbent Species Selection with Excess Gibbs Function. <i>Industrial & amp; Engineering Chemistry Research</i> , 2013 , 52, 9480-9489	.9	6
991	Solubility of hydrofluorocarbons in aromatic solvents and alcohols: Experimental data and modeling with CPA EoS. <i>Fluid Phase Equilibria</i> , 2013 , 337, 60-66	.5	8
990	Concentration dependent surface area parameter model for calculation of activity coefficients. Fluid Phase Equilibria, 2013 , 337, 165-173	.5	7
989	A revised LIQUAC and LIFAC model (LIQUAC*/LIFAC*) for the prediction of properties of electrolyte containing solutions. <i>Fluid Phase Equilibria</i> , 2013 , 337, 311-322	.5	38
988	Thermodynamics of alkanone+aromatic hydrocarbon mixtures. <i>Fluid Phase Equilibria</i> , 2013 , 337, 125-1362	.5	13
987	Experimental and VTPR-predicted volumetric properties of branched hexanes. <i>Fluid Phase Equilibria</i> , 2013 , 338, 141-147	.5	5
986	ThermoData Engine (TDE): software implementation of the dynamic data evaluation concept. 8. Properties of material streams and solvent design. 2013 , 53, 249-66		25
985	Rational function ridge regression in kinetic modeling: A case study. 2013 , 120, 136-141		6
984	MOQUAC, a new expression for the excess Gibbs energy based on molecular orientations. <i>Fluid Phase Equilibria</i> , 2013 , 338, 63-77	.5	9
983	Excess Mixture Properties and Activity Coefficients. 2013 , 271-349		
982	Selective Hydroalkoxylation of 1-Hexene with 1-Propanol and 1-Butanol over Zeolite Beta Catalyst. 2013 , 5, 576-581		9
981	Isobaric vaporliquid equilibrium for binary system of ethyl myristate+ethyl palmitate at 0.5, 1.0 and 1.5kPa. <i>Fluid Phase Equilibria</i> , 2013 , 347, 8-14	.5	13
980	Solubilities of selected organic electronic materials in pressurized hot water and estimations of aqueous solubilities at 298.15 K. 2013 , 90, 2035-40		6

	Accurate pre-calculation of limiting activity coefficients by COSMO-RS with molecular-class based parameterization. <i>Fluid Phase Equilibria</i> , 2013 , 340, 11-14	2.5	5
978	Peculiar features of four enzymes of the CaLA superfamily in aqueous media: Differences in substrate specificities and abilities to catalyze alcoholysis. 2013 , 94, 36-46		22
977	Measurements of the sensitivity of aerosol hygroscopicity and the [parameter to the O/C ratio. 2013, 117, 14120-31		80
976	Measurement of VLE data of carbon dioxide (CO2)+methyl iodide (CH3I) system for the direct synthesis of dimethyl carbonate using supercritical CO2 and methanol. 2013 , 81, 7-14		6
975	Mass transfer of hydroxyethyl cellulose membranes for desulfurization of FCC gasoline: Experimental and modeling. 2013 , 231, 255-261		11
974	Kinetic study of biphasic aldol condensation of n-butyraldehyde using stirred cell. 2013 , 104, 619-629		8
973	Surface study of binary mixtures containing chlorinated and oxygenated compounds. 2013, 181, 1-7		22
972	Solubilities of Isophthalic Acid in Acetic Acid + Water Solvent Mixtures. 2013 , 21, 754-758		6
971	An extensible framework for capturing solvent effects in computer generated kinetic models. 2013 , 117, 2955-70		23
970	Measurement and prediction of binary mixture flash point. 2013 , 11, 57-62		15
969	Measurement and prediction of binary mixture flash point. 2013 , 11, 57-62 Flash point of organic binary mixtures containing alcohols: experiment and prediction. 2013 , 11, 388-39	3	3
		2.5	
969	Flash point of organic binary mixtures containing alcohols: experiment and prediction. 2013 , 11, 388-39 Molecular structure-based methods of property prediction in application to lipids: A review and		3
969	Flash point of organic binary mixtures containing alcohols: experiment and prediction. 2013 , 11, 388-39 Molecular structure-based methods of property prediction in application to lipids: A review and refinement. <i>Fluid Phase Equilibria</i> , 2013 , 357, 2-18		3
969 968 967	Flash point of organic binary mixtures containing alcohols: experiment and prediction. 2013 , 11, 388-39 Molecular structure-based methods of property prediction in application to lipids: A review and refinement. <i>Fluid Phase Equilibria</i> , 2013 , 357, 2-18 Hydrate phase equilibria of furan, acetone, 1,4-dioxane, TBAC and TBAF. 2013 , 64, 151-158 Prediction of the solubility of selected pharmaceuticals in water and alcohols with a group		3 30 33
969 968 967 966	Flash point of organic binary mixtures containing alcohols: experiment and prediction. 2013 , 11, 388-39 Molecular structure-based methods of property prediction in application to lipids: A review and refinement. <i>Fluid Phase Equilibria</i> , 2013 , 357, 2-18 Hydrate phase equilibria of furan, acetone, 1,4-dioxane, TBAC and TBAF. 2013 , 64, 151-158 Prediction of the solubility of selected pharmaceuticals in water and alcohols with a group contribution method. 2013 , 62, 118-129 Prediction Model for the Odor Intensity of Fragrance Mixtures: A Valuable Tool for Perfumed	3.9	3 30 33 6
969 968 967 966	Flash point of organic binary mixtures containing alcohols: experiment and prediction. 2013, 11, 388-39 Molecular structure-based methods of property prediction in application to lipids: A review and refinement. Fluid Phase Equilibria, 2013, 357, 2-18 Hydrate phase equilibria of furan, acetone, 1,4-dioxane, TBAC and TBAF. 2013, 64, 151-158 Prediction of the solubility of selected pharmaceuticals in water and alcohols with a group contribution method. 2013, 62, 118-129 Prediction Model for the Odor Intensity of Fragrance Mixtures: A Valuable Tool for Perfumed Product Design. Industrial & Design Chemistry Research, 2013, 52, 963-971 Measurement and Modeling of Vapor Diguid Equilibria for Systems Containing Alcohols, Water, and	3.9	3 30 33 6 14

961	Prediction of Flash Points for Fuel Mixtures Using Machine Learning and a Novel Equation. 2013 , 27, 3811-3820	44
960	Extension of modified UNIFAC (Dortmund) matrix to piperidinium ionic liquids. <i>Fluid Phase Equilibria</i> , 2013 , 353, 115-120	18
959	Prediction of vaporllquid equilibria of binary systems containing esters by using Wilson equation with parameters estimated from pure-component properties. <i>Fluid Phase Equilibria</i> , 2013 , 352, 114-117	6
958	Volumetric study of the mixtures n-hexane + isomeric chlorobutane: experimental characterization and volume translated Peng-Robinson predictions. 2013 , 117, 10284-92	4
957	Experimental and Predicted Viscosities of Binary Mixtures Containing Chlorinated and Oxygenated Compounds. 2013 , 34, 34-46	13
956	Volatility of organic aerosol: evaporation of ammonium sulfate/succinic acid aqueous solution droplets. 2013 , 47, 12123-30	17
955	Investigating the impact of aqueous-phase chemistry and wet deposition on organic aerosol formation using a molecular surrogate modeling approach. 2013 , 47, 914-22	16
954	Experimental Study of Sorption and Diffusion of n-Pentane in Polystyrene. <i>Journal of Chemical & Engineering Data</i> , 2013 , 58, 851-865	11
953	Quantification of Carboxylic and Carbonyl Functional Groups in Organic Aerosol Infrared Absorbance Spectra. 2013 , 47, 310-325	68
952	Cloud droplet number enhanced by co-condensation of organic vapours. 2013, 6, 443-446	90
951	QSAR/QSPR Model Research of Complicated Samples. 2013 , 740, 306-309	
950	Comparisons between Hygroscopic Measurements and UNIFAC Model Predictions for Dicarboxylic Organic Aerosol Mixtures. 2013 , 2013, 1-9	1
949	Resource-Efficient Process Technology for Energy Plants. 2013 , 85, 1282-1289	4
948	A model to predict the permeation kinetics of dimethyl sulfoxide in articular cartilage. 2013 , 11, 51-6	3
947	Mass-based hygroscopicity parameter interaction model and measurement of atmospheric aerosol water uptake. 2013 , 13, 717-740	50
946	Model for acid-base chemistry in nanoparticle growth (MABNAG). 2013 , 13, 12507-12524	39
945	Modeling secondary organic aerosol in an urban area: application to Paris, France. 2013, 13, 983-996	52
944	Chemical and hygroscopic properties of aerosol organics at Storm Peak Laboratory. 2013 , 118, 4767-4779	25

943	Solid-liquid equilibrium of triolein with fatty alcohols. 2013 , 30, 33-43	28
942	Assessing the reliability of predictive activity coefficient models for molecules consisting of several functional groups. 2013 , 30, 1-11	26
941	Extension of LIR Equation of State to Alkylamines Using Group Contribution Method. 2013 , 2013, 1-9	
940	The thermodynamics of alcohols-hydrocarbons mixtures. 2013 , 3, 01018	
939	Simulation of Extractive Distillation for Recycling Tetrahydrofuran from Pharmaceutical Wastewater with Chem CAD Software. 2013 , 5, 4769-4774	
938	Thermodynamics of water sorption in high performance glassy thermoplastic polymers. 2014 , 2, 25	12
937	Molecules Matter. 2014 , 55-64	27
936	Assessing the use of NMR chemical shifts for prediction of VLE in non-ideal binary liquid mixtures. 2014 , 119, 331-333	1
935	Liquid[liquid Equilibria of Water + 1-Butanol + Amino Acid (Glycine or dl-Alanine or l-Leucine) at 313.15 K. 2014 , 43, 2101-2116	3
934	Group contribution methodology based on the statistical associating fluid theory for heteronuclear molecules formed from Mie segments. 2014 , 140, 054107	174
933	Calculation on phase diagrams of polyetherimide/N,N-dimethylacetamide/H2O-BuOH casting system and their relevance to membrane performances. 2014 , 8, 312-319	2
932	Application of COSMO-RS Method for the Prediction of Liquid-Liquid Equilibrium of Water/n-Dodecane/1-Butanol. 2014 , 2014, 1-6	3
931	Calculating osmotic pressure of xylitol solutions from molality according to UNIFAC model and measuring it with air humidity osmometry. 2014 , 19, 853-5	1
930	Optimal Experimental Design for the Characterization of Liquid Liquid Equilibria. <i>Industrial & amp; Engineering Chemistry Research</i> , 2014 , 53, 19620-19627	11
929	Excess molar enthalpies for binary mixtures of n-propanol, acetic acid, and n-propyl acetate at 313.15 K and atmospheric pressure. <i>Fluid Phase Equilibria</i> , 2014 , 381, 77-82	10
928	Viscosities and densities of systems containing fatty compounds and alcoholic solvents. 2014 , 92, 1939-1950	5
927	The use of COSMO-SAC to predict relative adhesion between polymer matrices and silane-treated glass surfaces in filled particulate composites. 2014 , 28, 1312-1322	1
926	Henry's law constants of polyols. 2014 , 14, 12815-12837	8

925	Silanol-Assisted Aldol Condensation on Aminated Silica: Understanding the Arrangement of Functional Groups. 2014 , 6, 255-264	38
924	Reaction Kinetics of Catalytic Esterification of Nonanoic Acid with Ethanol over Amberlyst 15. 2014 , 12, 451-463	12
923	Prediction of physical properties for molecular design of solvents. <i>Fluid Phase Equilibria</i> , 2014 , 362, 74-80.5	11
922	PC-SAFT parameters from ab initio calculations. <i>Fluid Phase Equilibria</i> , 2014 , 362, 41-50 2.5	21
921	Statistical mechanical theory of fluid mixtures. 2014 , 393, 62-75	3
920	Evaluation of optimal activity coefficient models for modeling and simulation of liquid l lquid equilibrium of biodiesel + glycerol + alcohol systems. 2014 , 125, 57-65	23
919	Towards automated characterisation of liquid II quid equilibria. Fluid Phase Equilibria, 2014, 362, 328-334 2.5	7
918	Quantitative NMR spectroscopy of binary liquid mixtures (aldehyde+alcohol). Part III: (1-decanal or 3-phenylpropanal or 2-chlorobenzaldehyde)+(methanol or ethanol or 1-propanol). 2014 , 77, 167-177	
917	An algorithm for the regression of the UNIQUAC interaction parameters in liquid I quid equilibrium for single- and multi-temperature experimental data. Fluid Phase Equilibria, 2014, 374, 79-85	3
916	A short note on the use of an equation of state (EOS) based approach to modelling the thermodynamics of biodiesel systems. 2014 , 121, 70-75	2
915	Liquid II quid equilibrium data and thermodynamic modeling, at T/K=298.2, in the washing step of ethyl biodiesel production from crambe, fodder radish and macauba pulp oils. 2014 , 117, 590-597	23
914	Measurement and correlation of the solubilities of tetra(5,5-dimethyl-1,3-dioxaphosphorinanyl-2-oxy) neopentane in different pure solvents. <i>Fluid</i> 2.5 <i>Phase Equilibria</i> , 2014 , 367, 117-124	19
913	Ternary phase diagrams for aqueous mixtures of butyric acid with several solvents: Experimental and correlated data. <i>Fluid Phase Equilibria</i> , 2014 , 371, 50-56	6
912	Separation of Acylglycerides Obtained by Enzymatic Esterification Using Solvent Extraction. 2014 , 91, 261-270	3
911	Atmospheric and Aerosol Chemistry. 2014 ,	21
910	Chemical Thermodynamics: A Journey of Many Vistas. 2014 , 43, 525-576	11
909	(Solid + liquid) phase equilibria and heat capacity of (diphenyl ether + biphenyl) mixtures used as thermal energy storage materials. 2014 , 74, 43-50	28
908	Experiments and thermodynamic models for ternary (liquid[]quid) equilibrium systems of water+cyclopentanone+organic solvents at T=298.2K. 2014 , 196, 98-106	15

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907	Isothermal vaporlīquid equilibrium and excess molar enthalpies of the binary mixtures furfural+methyl isobutyl ketone, +2-butanol and +2-methyl-2-butanol. <i>Fluid Phase Equilibria</i> , 2014 , 372, 85-99	2.5	9
906	Modelling the distribution of a(w), pH and ions in marinated beef meat. 2014, 97, 347-57		15
905	Hybrid separations combining distillation and organic solvent nanofiltration for separation of wide boiling mixtures. 2014 , 92, 2131-2147		30
904	A new hydrogen bonding local composition based model in obtaining phase behavior of aqueous solutions of sugars. 2014 , 195, 47-53		14
903	Kinetic study of competitive catalytic transfer hydrogenation on a multi-functional molecule: 4-benzyloxy-4?-chlorochalcone. 2014 , 111, 1-14		2
902	Amberlyst 15 Catalyzed Esterification of Nonanoic Acid with 1-Propanol: Kinetics, Modeling, and Comparison of Its Reaction Kinetics with Lower Alcohols. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 2167-2174	3.9	39
901	Evaluation of COSMO-RS model in binary and ternary mixtures of natural antioxidants, ionic liquids and organic solvents. <i>Fluid Phase Equilibria</i> , 2014 , 369, 55-67	2.5	19
900	Data, analysis and modeling of physical properties for process design of systems involving lipids. <i>Fluid Phase Equilibria</i> , 2014 , 362, 318-327	2.5	22
899	Correlation of phase equilibria for the systems containing 1-butanol+water by concentration dependent surface area parameter model. <i>Fluid Phase Equilibria</i> , 2014 , 362, 35-40	2.5	
898	Kinetics of non-catalytic and ZnL2-catalyzed esterification of lauric acid with ethanol. 2014 , 117, 125-	132	23
897	Diffusion and solubility of hazardous compounds in polyvinyl chloride. <i>Fluid Phase Equilibria</i> , 2014 , 366, 69-73	2.5	3
896	Development and analysis of the Original UNIFAC-CI model for prediction of vaporliquid and solidliquid equilibria. <i>Fluid Phase Equilibria</i> , 2014 , 366, 24-44	2.5	6
895	Liquid II quid equilibrium of the CuSO4+PEG 4000+H2O system at different temperatures. <i>Fluid Phase Equilibria</i> , 2014 , 363, 199-206	2.5	23
894	Isobaric vaporllquid equilibrium for binary system of cinnamaldehyde+benzaldehyde at 10, 20 and 30kPa. <i>Fluid Phase Equilibria</i> , 2014 , 364, 62-66	2.5	11
893	Simultaneous correlation of infinite dilution activity coefficient, vapor []quid, and liquid []quid equilibrium data with F-SAC. Fluid Phase Equilibria, 2014, 364, 31-41	2.5	11
892	Extrapolation/interpolation of infinite dilution, activity coefficient as well as liquid and solid solubility between solvents: Part 1. Alkane solvents. <i>Fluid Phase Equilibria</i> , 2014 , 361, 69-82	2.5	6
891	1000 1 15 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1	- (85
	UNIFAC model for ionic liquid-CO2 systems. <i>AICHE Journal</i> , 2014 , 60, 716-729	3.6	

889	SOLVENT USE IN VARIOUS INDUSTRIES. 2014 , 1-261		O
888	Selection of Biphasic Liquid Systems in Liquid-Liquid Chromatography Using Predictive Thermodynamic Models. 2014 , 37, 1663-1674		18
887	Liquid Phase Equilibria of the Water + Acetic Acid + Dimethyl Carbonate Ternary System at Several Temperatures. <i>Journal of Chemical & Engineering Data</i> , 2014 , 59, 3353-3358	2.8	7
886	Cellulose and hemicellulose valorisation: an integrated challenge of catalysis and reaction engineering. 2014 , 7, 2803		219
885	Rapid Solvent Screening Using Thermodynamic Models for Recovery of 2,3-Butanediol from Fermentation by Liquid Liquid Extraction. <i>Journal of Chemical & Ch</i>	4 63 8	23
884	Prediction of Solubilities and Partition Coefficients in Polymers Using COSMO-RS. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 11478-11487	3.9	47
883	The Crystal-T algorithm: a new approach to calculate the SLE of lipidic mixtures presenting solid solutions. 2014 , 16, 16740-54		18
882	Succinic acid in aqueous solution: connecting microscopic surface composition and macroscopic surface tension. 2014 , 16, 21486-95		20
881	Liquid II quid equilibria of water+acetic acid+2-ethyl hexyl acetate ternary system. <i>Fluid Phase Equilibria</i> , 2014 , 379, 206-211	2.5	4
880	Effect of the cation on the interactions between alkyl methyl imidazolium chloride ionic liquids and water. 2014 , 118, 10503-14		51
879	Vaporliquid Equilibrium and Physical Properties for Distillation. 2014 , 45-95		1
878	Solubility and Solubility Modeling of Polycyclic Aromatic Hydrocarbons in Subcritical Ethanol and Water Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 10238-10248	3.9	11
877	Liquid Diquid Phase Equilibria for Soybean Oil Methanolysis: Experimental, Modeling, and Data Prediction. <i>Industrial & Digineering Chemistry Research</i> , 2014 , 53, 3731-3736	3.9	14
876	Extractive distillation with ionic liquids: A review. AICHE Journal, 2014, 60, 3312-3329	3.6	215
875	Volatile Hydrocarbons and Fuel Oxygenates. 2014 , 439-480		4
874	An Improvement to COSMO-SAC for Predicting Thermodynamic Properties. <i>Industrial & amp; Engineering Chemistry Research</i> , 2014 , 53, 8265-8278	3.9	65
873	Vapourliquid equilibrium of carboxylic acidlicohol binary systems: 2-Propanol+butyric acid, 2-butanol+butyric acid and 2-methyl-1-propanol+butyric acid. <i>Fluid Phase Equilibria</i> , 2014 , 380, 18-27	2.5	4
872	Prediction of Thermodynamic Properties and Phase Behavior of Fluids and Mixtures with the SAFT-∰Mie Group-Contribution Equation of State. <i>Journal of Chemical & Data</i> , 2014, 59, 3272-3288	2.8	82

871	The Use of Acid-Activated Montmorillonite as a Solid Catalyst for the Production of Fatty Acid Methyl Esters. 2014 , 28, 5834-5840		13
870	Simulation, optimization, and sensitivity analysis of a natural gas dehydration unit. 2014 , 21, 159-169		34
869	Preface to the Memorial Edition for Grant M. Wilson. <i>Journal of Chemical & Data</i> , 2014, 59, 943-945	2.8	1
868	Equilibrium Speciation in Moderately Concentrated FormaldehydeMethanolWater Solutions Investigated Using 13C and 1H Nuclear Magnetic Resonance Spectroscopy. <i>Industrial & amp; Engineering Chemistry Research</i> , 2014 , 53, 9262-9271	3.9	25
867	Miscibility of ternary systems containing kerosene-based surrogate fuel and hydrous ethanol: Experimental data + thermodynamic modeling. <i>Fluid Phase Equilibria</i> , 2014 , 379, 1-9	2.5	9
866	Liquid¶quid equilibria of water + lactic acid + methyl isobutyl ketone. <i>Fluid Phase Equilibria</i> , 2014 , 379, 19-25	2.5	3
865	Isothermal vaporliquid equilibria for the binary system of dimethyl ether (DME)+methyl iodide (CH3I). Fluid Phase Equilibria, 2014 , 379, 52-58	2.5	3
864	Solid[liquid Phase Equilibria of N,N?-[1,3-Phenylenebis(methylene)]bis(phosphoramidic acid) P,P,P?-Tetraphenyl Ester in 10 Pure Solvents. <i>Journal of Chemical & Data, 2014,</i> 59, 1533-1539	2.8	5
863	Vapor l lquid equilibrium for propylene glycols binary systems: Experimental data and regression. <i>Fluid Phase Equilibria</i> , 2014 , 382, 244-253	2.5	6
862	Algorithmic Framework for Quality Assessment of Phase Equilibrium Data. <i>Journal of Chemical</i> & Samp; Engineering Data, 2014 , 59, 2283-2293	2.8	27
861	Conceptual Design of Flowsheet Options Based on Thermodynamic Insights for (Reaction) Separation Processes Applying Process Intensification. <i>Industrial & Design Engineering Chemistry Research</i> , 2014 , 53, 13412-13429	3.9	18
860	A Review of Flash Point Prediction Models for Flammable Liquid Mixtures. <i>Industrial & amp; Engineering Chemistry Research</i> , 2014 , 53, 12553-12565	3.9	46
859	Solubility calculations of branched and linear amino acids using lattice cluster theory. 2014 , 112, 2282-2	296	10
858	A Priori Prediction of the Vaporlliquid Equilibria of Mixtures of Acetic Acid and Water or Alcohols by Explicit Consideration of Hydrogen-Bonded Dimers. <i>Industrial & Dimers </i>	3.9	4
857	Excess molar volumes and excess molar enthalpies in binary systems N-alkyl-triethylammonium bis(trifluoromethylsulfonyl)imide+methanol. <i>Fluid Phase Equilibria</i> , 2014 , 363, 156-166	2.5	17
856	COSMO-RS-PDHS: A new predictive model for aqueous electrolytes solutions. 2014 , 92, 2873-2883		21
855	Improving GC-PPC-SAFT equation of state for LLE of hydrocarbons and oxygenated compounds with water. <i>Fluid Phase Equilibria</i> , 2014 , 372, 113-125	2.5	16
854	Phase equilibria of systems containing aromatic oxygenated compounds with CH4, CO2, H2, H2S, CO and NH3: Experimental data and predictions. <i>Fluid Phase Equilibria</i> , 2014 , 382, 219-234	2.5	3

853	Phase Equilibria. 2014 , 35, 201-251		4
852	Selection of Solvents with A-UNIFAC Applied to Detoxification of Aqueous Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2014 , 53, 17051-17058	3.9	6
851	Isomer effect of propanol on liquid[Iquid equilibrium in hydrophobic room-temperature ionic liquids. 2014 , 613, 122-126		15
850	Influence of functional groups on organic aerosol cloud condensation nucleus activity. 2014 , 48, 10182-	90	79
849	Phase Equilibrium of Binary Mixtures of n-Hexane + Branched Chlorobutanes: Experimental Results and Group Contribution Predictions. <i>Journal of Chemical & Engineering Data</i> , 2014 , 59, 3017-3024	2.8	4
848	Liquid Phase Equilibria of Water + Formic Acid + Dimethyl Carbonate Ternary System at Several Temperatures. <i>Journal of Chemical & Data</i> , 2014, 59, 2781-2787	2.8	14
847	Vapor-Liquid Equilibrium Prediction of Ammonia-Ionic Liquid Working Pairs of Absorption Cycle Using UNIFAC Model. 2014 , 22, 72-78		18
846	(Solid+liquid) solubility of organic compounds in organic solvents ©orrelation and extrapolation. 2014 , 76, 124-133		19
845	Quantitative NMR spectroscopy of binary liquid mixtures (aldehyde + alcohol) Part I: Acetaldehyde + (methanol or ethanol or 1-propanol). 2014 , 68, 332-342		4
844	Ternary (liquid l iquid) equilibrium data of furfuryl alcohol with organic solvents at T=298.2K: Experimental results and thermodynamic models. <i>Fluid Phase Equilibria</i> , 2014 , 365, 88-96	2.5	21
843	Thermostabilities and solubilities of flame retardant bisphenol S-bis (5,5-dimethyl-1,3-dioxaphosphorinanyl-2-oxy phosphate ester) as a function of temperature. <i>Fluid Phase Equilibria</i> , 2014 , 373, 55-62	2.5	2
842	Separation of ethyl acetateßooctane mixture by heteroazeotropic batch distillation. 2014 , 92, 995-100-	1	9
841	Computer-aided screening of solvents for optimal reaction rates. 2014 , 115, 167-176		8
840	Reprint of "Quantitative NMR spectroscopy of binary liquid mixtures (aldehyde+alcohol). Part II: (Propanal or butanal or heptanal)+(methanol or ethanol or 1-propanol)". 2014 , 68, 343-356		1
839	On the solid I Iquid equilibrium of binary mixtures of fatty alcohols and fatty acids. <i>Fluid Phase Equilibria</i> , 2014 , 366, 88-98	2.5	50
838	Trends and demands in the solid[Iquid equilibrium of lipidic mixtures. 2014 , 4, 31840-31850		28
837	A review of imidazolium ionic liquids research and development towards working pair of absorption cycle. 2014 , 37, 47-68		147
836	Solubility of nonelectrolytes: a first-principles computational approach. 2014 , 118, 5194-202		11

(2015-2014)

835	Calculation of Henry's law constants for some volatile organic compounds dissolved in aqueous Na2SO4 and NaCl solutions using the LIFAC activity coefficient model. <i>Fluid Phase Equilibria</i> , 2014 , 376, 96-104	1
834	Simultaneous liquid I quid and vapour I quid equilibria predictions of selected oxygenated aromatic molecules in mixtures with alkanes, alcohols, water, using the polar GC-PC-SAFT. 2014 , 92, 2912-293	35 ²¹
833	Flash-point estimation for binary partially miscible mixtures of flammable solvents by UNIFAC group contribution methods. <i>Fluid Phase Equilibria</i> , 2014 , 375, 275-285	20
832	Conversion of microalgae to jet fuel: process design and simulation. 2014 , 167, 349-57	19
831	Isobaric (vapor + liquid) equilibrium data for the binary system methanol + 2-butyl alcohol and the quaternary system methyl acetate + methanol + 2-butyl alcohol + 2-butyl acetate at $P = 101.33 \text{ kPa}$. 2014 , 74, 85-90	7
830	Synthesis of dimethyl carbonate and propylene glycol in a membrane-assisted reactive distillation process: Pilot-scale experiments, modeling and process analysis. 2014 , 84, 54-70	30
829	Optimization-Based Approaches to Computational Molecular Design. 2014 , 173-193	
828	Molecular Modeling of Formulated Consumer Products. 2014 , 195-206	
827	Computer-Aided Methodologies for the Design of Reaction Solvents. 2014 , 267-305	
826	Prediction of Vaporliquid Equilibria of Binary Systems at Reduced Pressures by Using Wilson Equation with Parameters Estimated from Pure-Component Properties. 2014 , 47, 10-13	2
825	Chapter 4MATLABfi for Chemical Engineering. 2014 , 105-176	1
824	Group Contribution Methodologies for the Prediction of Thermodynamic Properties and Phase Behavior in Mixtures. 2014 , 135-172	1
823	Hygroscopicity of organic compounds from biomass burning and their influence on the water uptake of mixed organic ammonium sulfate aerosols. 2014 , 14, 11165-11183	33
822	Experimental determination of the temperature dependence of water activities for a selection of aqueous organic solutions. 2014 , 14, 9993-10012	16
821	Henry's law constants of diacids and hydroxy polyacids: recommended values. 2014 , 14, 2699-2712	17
820	Computational Prediction of Solvent and Surfactant Properties Using the Conductor-Like Screening Model (COSMO) For Chemical Enhanced Oil Recovery Research. 2014 ,	Ο
819	Pressurized hot water extraction of polyphenols from plant material. 2015 , 63-101	3
818	Molecular Thermodynamics of Hydrogen-Bonded Systems. 2015 , 145-198	

817	Tears of wine: new insights on an old phenomenon. 2015 , 5, 16162		36
816	Modeling of PVT-Properties of Natural Gas Condensate Mixtures Adjusted for Presence of Residual Water in Collector (Russian). 2015 ,		
815	Flash Points of Secondary Alcohol and n-Alkane Mixtures. 2015 , 119, 14697-704		2
814	Solvent effects on esterification equilibria. <i>AICHE Journal</i> , 2015 , 61, 3000-3011	3.6	21
813	Molecular thermodynamics of LNA:LNA base pairs and the hyperstabilizing effect of 5?-proximal LNA:DNA base pairs. <i>AICHE Journal</i> , 2015 , 61, 2711-2731	3.6	4
812	Improved AIOMFAC model parameterisation of the temperature dependence of activity coefficients for aqueous organic mixtures. 2015 , 15, 447-493		31
811	Describing the sorption characteristics of a ternary system of benzene (1) and alcohol (2) in a nonporous polymer membrane (3) by the FloryHuggins model. 2015 , 55, 1187-1195		4
810	Modeling of PVT-Properties of Natural Gas Condensate Mixtures Adjusted for Presence of Residual Water in Collector. 2015 ,		
809	Thermodynamic and kinetic study of the production of oxygenated compounds: Synthesis of 1,1-diethoxybutane catalyzed by amberlyst-15. 2015 , 93, 1990-1998		5
808	A generalized procedure for the prediction of multicomponent adsorption equilibria. <i>AICHE Journal</i> , 2015 , 61, 2600-2610	3.6	4
807	Analysis of countercurrent membrane vapor extraction of a dilute aqueous biosolute. <i>AICHE Journal</i> , 2015 , 61, 2795-2809	3.6	10
806	The universal recovery strategy. 2015 , 59-81		6
805	The Effect of Non-Ideal Vapour-Liquid Equilibrium and Non-Ideal Liquid Diffusion on Multi-Component Droplet Evaporation for Gasoline Direct Injection Engines. 2015 ,		4
804	Prediction of Solubility of Active Pharmaceutical Ingredients in Single Solvents and Their Mixtures Bolvent Screening. 2015 ,		
803	Tailor-Made Green Diesel Blends Design using a Decomposition-Based Computer-Aided Approach. 2015 , 1085-1090		7
802	Combining mixing rules with QSPR models for pure chemicals to predict the flash points of binary organic liquid mixtures. 2015 , 74, 61-70		20
801	Experimental Study on Condensation Heat Transfer of Ethanol Water Vapor Mixtures on Vertical Micro-tubes. 2015 , 36, 1598-1617		1
800	Removal of thiophene from n-heptane/thiophene mixtures by spiral wound pervaporation module: Modelling, validation and influence of operating conditions. 2015 , 490, 328-345		24

799 Sequential Centrifugal Partition Chromatography. **2015**, 245-272

798	Experimental investigation and thermodynamic modeling of wax disappearance temperature for n-undecane + n-hexadecane + n-octadecane and n-tetradecane + n-hexadecane + n-octadecane ternary systems. Fluid Phase Equilibria, 2015, 403, 70-77	2.5	8
797	New modified UNIFAC parameters using critically evaluated phase equilibrium data. <i>Fluid Phase Equilibria</i> , 2015 , 388, 128-141	2.5	42
796	Technical equation of state models for heat transfer fluids made of biphenyl and diphenyl ether and their mixtures. <i>Fluid Phase Equilibria</i> , 2015 , 393, 64-77	2.5	5
795	The UNIFAC model and the partition of alkyl and alkylphenol ethoxylate surfactants in the excess phases of middle phase microemulsions. <i>Fluid Phase Equilibria</i> , 2015 , 397, 117-125	2.5	15
794	Separation of ethylbenzene and n-octane using deep eutectic solvents. 2015 , 4,		5
793	The Secondary Organic Aerosol Processor (SOAP v1.0) model: a unified model with different ranges of complexity based on the molecular surrogate approach. 2015 , 8, 1111-1138		38
792	Influence of organic compound functionality on aerosol hygroscopicity: dicarboxylic acids, alkyl-substituents, sugars and amino acids. 2017 , 17, 5583-5599		43
791	Predicting Critical Micelle Concentrations with Molecular Dynamics Simulations and COSMOmic. 2017 , 89, 1288-1296		10
790	Comparison of Direct-Injection Spray Development of E10 Gasoline to a Single and Multi-Component E10 Gasoline Surrogate. 2017 , 10, 352-368		3
789	A Systematic Identification Method for Thermodynamic Property Modelling. 2017 , 40, 205-210		
788	Maxwell-Stefan diffusion: a framework for predicting condensed phase diffusion and phase separation in atmospheric aerosol. 2017 ,		
787	Ozonolysis of <i></i>-phellandrene, Part 1: Gas- and particle-phase characterisation. 2017 ,		
786	From Wilson to F-SAC: A comparative analysis of correlative and predictive activity coefficient models to determine VLE and IDAC of binary systems. <i>Fluid Phase Equilibria</i> , 2018 , 464, 1-11	2.5	4
785	Interpretation of cytochrome P450 monooxygenase kinetics by modeling of thermodynamic activity. 2018 , 183, 172-178		6
784	Solubility prediction of naphthalene in carbon dioxide from crystal microstructure. 2018 , 148, 094109		1
783	Two-Phase Flow in Liquid Chromatography, Part 1: Experimental Investigation and Theoretical Description. <i>Industrial & Description</i> . <i>Industrial & Description</i> . <i>Industrial & Description</i> .	3.9	3
782	Predicting Limiting Activity Coefficients and Phase Behavior from Molecular Structure: Expanding MOSCED to Alkanediols Using Group Contribution Methods and Electronic Structure Calculations. <i>Journal of Chemical & Data</i> , 2018, 63, 2586-2598	2.8	10

781	Measurement and Correlation of Isobaric Vaporlliquid Equilibrium for Binary Systems of Allyl Alcohol with Isobutyl Acetate, Butyl Acetate, and Butyl Propionate at 101.3 kPa. <i>Journal of Chemical & Data</i> , 2018, 63, 845-852	2.8	7
780	Review and Thermodynamic Modeling with NRTL Model of Vaporliquid Equilibria (VLE) of Aroma Compounds Highly Diluted in Ethanoll Water Mixtures at 101.3 kPa. <i>Industrial & amp; Engineering Chemistry Research</i> , 2018 , 57, 3443-3470	3.9	14
779	Prediction of Physicochemical Properties of Compounds. 2018 , 53-81		3
778	Condensation heat transfer correlation for water-ethanol vapor mixture flowing through a plate heat exchanger. 2018 , 54, 3025-3033		5
777	MaxwellBtefan diffusion: a framework for predicting condensed phase diffusion and phase separation in atmospheric aerosol. 2018 , 18, 1629-1642		10
776	Description of Adsorption in Liquid Chromatography under Nonideal Conditions. 2018 , 34, 5655-5671		4
775	Effect of Heterogeneous Chemical Reactions on the KI liler Activation of Aqueous Organic Aerosols. 2018 , 122, 4322-4337		6
774	A theoretically based departure function for multi-fluid mixture models. <i>Fluid Phase Equilibria</i> , 2018 , 469, 56-69	2.5	9
773	Influence of Cosolutes on Chemical Equilibrium: a Kirkwood B uff Theory for Ion Pair Association D issociation Processes in Ternary Electrolyte Solutions. 2018 , 122, 10293-10302		20
772	Computer aided chemical product design [ProCAPD and tailor-made blended products. 2018 , 116, 37-5	5	36
771	Kinetics Study and Parametric Sensitivity Analysis of Esterification of Butyric Acid with Benzyl Alcohol: A Taguchi Methodology Approach. 2018 , 16,		1
770	Purification of Monoglycerides From Palm Stearin by Liquid[liquid Extraction With Aqueous Ethanol. 2018 , 95, 217-228		2
769	Kinetics of esterification of benzoic acid and isoamyl alcohol catalyzed by P-toluenesulphonic acid. 2018 , 96, 2443-2449		2
768	Vapor - liquid equilibrium of the carbon dioxide/methane mixture at three isotherms. <i>Fluid Phase Equilibria</i> , 2018 , 462, 44-58	2.5	9
767	Minimum flash point behavior of ternary solutions with three minimum flash point binary constituents. 2018 , 217, 626-632		5
766	Measurement and thermodynamic modelling of ternary liquid-liquid equilibrium for extraction of (1R,2R)-()11,2-Diaminocyclohexane from aqueous solution with C405 alcohols at different temperatures. 2018, 120, 184-190		8
765	Flash point of flammable binary mixtures: Synergistic behavior. 2018 , 52, 1-6		21
764	Estimation of MOSCED parameters from the COSMO-SAC database. <i>Fluid Phase Equilibria</i> , 2018 , 470, 241-248	2.5	8

763	The design of optimal mixtures from atom groups using Generalized Disjunctive Programming. 2018 , 116, 401-421		16
762	Equilibrium data and thermodynamic studies of https://examplese.partition in aqueous two-phase systems. Fluid Phase Equilibria, 2018, 463, 69-79	2.5	11
761	Early process development of API applied to poorly water-soluble TBID. 2018, 126, 2-9		1
760	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 & Description of State (State of State o</i>	3.9	10
759	Infinite dilution activity coefficient from SMD calculations: accuracy and performance for predicting liquid-liquid equilibria. 2018 , 24, 56		8
75 ⁸	Impact of impurities on CO 2 storage in saline aquifers: Modelling of gases solubility in water. 2018 , 68, 247-255		12
757	Effects of aromatic fluids on properties and stability of alternative marine diesels. 2018 , 216, 171-180		6
756	Systematic Optimization-Based Integrated Chemical Product P rocess Design Framework. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 677-688	3.9	16
755	Kinetics of homogeneous and heterogeneous reactions in the reductive aminolysis of glucose with dimethylamine. 2018 , 227, 161-169		8
754	CO2 capture by methanol, ionic liquid, and their binary mixtures: Experiments, modeling, and process simulation. <i>AICHE Journal</i> , 2018 , 64, 2168-2180	3.6	38
753	Analysis of temperature glide matching of heat pumps with zeotropic working fluid mixtures for different temperature glides. 2018 , 153, 650-660		36
75²	Extension of HLD-NAC Flash Calculation Algorithm to Multicomponent Mixtures of Microemulsion and Excess Phases. 2018 ,		4
751	Impact of higher order diagrams on phase equilibrium calculations for small molecules using lattice cluster theory. 2018 , 148, 094103		2
75 ⁰	Hygroscopicity of organic surrogate compounds from biomass burning and their effect on the efflorescence of ammonium sulfate in mixed aerosol particles. 2018 , 18, 1045-1064		16
749	Thermodynamics of mixtures containing a very strongly polar compound. 12. Systems with nitrobenzene or 1-nitroalkane and hydrocarbons or 1-alkanols. <i>Fluid Phase Equilibria</i> , 2018 , 471, 24-39	2.5	6
748	Thermodynamic modeling of amino acid solutions: A new perspective on CPA EOS. 2018 , 124, 21-31		3
747	An open and extensible sigma-profile database for COSMO-based models. AICHE Journal, 2018, 64, 344.	333455	 5 28
746	Predictive method of hydrogen solubility in heavy petroleum fractions using EOS/GE and group contributions methods. 2018 , 224, 619-627		10

745	Biomass to levulinic acid: A techno-economic analysis and sustainability of biorefinery processes in Southeast Asia. 2018 , 214, 267-275		31
744	Systematic identification method for data analysis and phase equilibria modelling for lipids systems. 2018 , 121, 153-169		9
743	Cation-Exchange Resin Catalyzed Ketalization Reaction of Cyclohexanone with 1,4-Butanediol: Thermodynamics and Kinetics. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 4841-4847	3.9	8
742	On the calculation of nearest neighbors in activity coefficient models. <i>Fluid Phase Equilibria</i> , 2018 , 465, 10-23	2.5	6
741	Carbon capture and storage (CCS): the way forward. 2018, 11, 1062-1176		1368
740	Novel strategies for the formulation and processing of poorly water-soluble drugs. 2018 , 126, 40-56		73
739	Modeling food matrix effects on chemical reactivity: Challenges and perspectives. 2018 , 58, 2814-2828		32
738	COSMO-based computer-aided molecular/mixture design: A focus on reaction solvents. <i>AICHE Journal</i> , 2018 , 64, 104-122	3.6	25
737	Measurement and correlation of solid[Iquid phase equilibria for binary and ternary systems consisting of N -vinylpyrrolidone, 2-pyrrolidone and water. 2018 , 26, 806-811		6
736	Further development of the predictive models for physical properties of pure ionic liquids: Thermal conductivity and heat capacity. 2018 , 118, 1-15		30
735	Computer-aided design of ionic liquids as solvents for extractive desulfurization. <i>AICHE Journal</i> , 2018 , 64, 1013-1025	3.6	97
734	The correlation and prediction of the temperature variation of infinite dilution activity coefficients of compounds in water. <i>Fluid Phase Equilibria</i> , 2018 , 455, 1-5	2.5	4
733	Solubility of solvents in polyethylene below the melt temperature. Fluid Phase Equilibria, 2018, 470, 68-	7<u>4</u>5	6
732	Thermodynamic affinity-based considerations for the rational selection of biphasic systems for microbial flavor and fragrance production. 2018 , 93, 656-666		9
731	Measurement and correlation of isobaric vapourllquid equilibrium for systems of o-cresol, m-cresol and 2, 6-dimethylphenol at 20.0 kPa. <i>Fluid Phase Equilibria</i> , 2018 , 459, 44-50	2.5	6
730	Extending the range of COSMO-SAC to high temperatures and high pressures. <i>AICHE Journal</i> , 2018 , 64, 1806-1813	3.6	3
729	Microemulsion Phase-Behavior Equation-of-State Model Using Empirical Trends in Chemical Potentials. 2018 , 23, 819-830		7
728	Integrated reaction and separation in a continuous middle vessel column for enhancing indirect hydration of cyclohexene to cyclohexanol. 2018 , 123, 249-257		9

727	Model evaluation for the prediction of solubility of active pharmaceutical ingredients (APIs) to guide solid-liquid separator design. 2018 , 13, 265-278		6
726	Improvement of predictive tools for vapor-liquid equilibrium based on group contribution methods applied to lipid technology. <i>Fluid Phase Equilibria</i> , 2018 , 470, 249-258	2.5	7
725	The maximum flammable content for binary aqueous organic mixtures not to flash and their maximum flash points. <i>AICHE Journal</i> , 2018 , 64, 263-271	3.6	1
724	Modeling the effect of non-ideality, dynamic mass transfer and viscosity on SOA formation in a 3-D air quality model. 2018 ,		
723	LIQUID-LIQUID EQUILIBRIUM OF SYSTEMS COMPOSED OF SOYBEAN OIL + MONOACYLGLYCEROLS + DIACYLGLYCEROLS + ETHYL OLEATE + OLEIC ACID + ETHANOL AT 303.15 AND 318.15 K. 2018 , 35, 373-382		2
722	. 2018,		6
721	Absorption. 2018 , 1-115		О
720	. 2018,		2
719	Thermodynamic Modeling of Natural Gas and Gas Condensate Mixtures. 2018, 57-88		
718	Mitigating Complexity: Cohesion Parameters and Related Topics. I: The Hildebrand Solubility Parameter. 2018 , 47, 1626-1709		9
717	Strategies to Define Surrogate Fuels for the Description of the Multicomponent Evaporation Behavior of Hydrocarbon Fuels. 2018 ,		4
716	Synergistic Extraction of Hydroquinone from Aqueous Solution with Solvent Mixture of 2-Pentanone and n-Pentanol: Liquid[liquid Equilibria and Data Correlation. <i>Journal of Chemical & Engineering Data</i> , 2018 ,	2.8	3
715	Properties of Ion Complexes and Their Impact on Charge Transport in Organic Solvent-Based Electrolyte Solutions for Lithium Batteries: Insights from a Theoretical Perspective. 2018 , 4, 62		27
714	Isothermal Bubble Pressure Data for the Binary System of C2F6 and n-Octane. <i>Journal of Chemical</i> & Samp; Engineering Data, 2018 ,	2.8	
713	A critical review of the model fitting quality and parameter stability of equilibrium adsorption models. 2018 , 262, 50-68		18
712	Dampf-Fl Bsigkeits-Gleichgewichte von Mehrkomponenten-Gemischen. 2018 , 1-18		
711	Insights into Noncovalent Binding Obtained from Molecular Dynamics Simulations. 2018, 90, 1864-187	5	8
710	LIQUID-LIQUID EQUILIBRIA FOR SYSTEMS CONTAINING FATTY ACID ETHYL ESTERS, ETHANOL AND GLYCEROL AT 333.15 AND 343.15 K: EXPERIMENTAL DATA, THERMODYNAMIC AND ARTIFICIAL NEURAL NETWORK MODELING. 2018 , 35, 819-834		2

709	A United Chemical Thermodynamic Model: COSMO-UNIFAC. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 15954-15958	3.9	28
708	Thermodynamics of Physical and Chemical Transformations. 2018, 9-115		
707	Solubility and solid phase studies of isomeric phenolic acids in pure solvents. 2018 , 272, 1048-1057		12
706	Kinetic study of liquid phase esterification of lactic acid with n-amyl alcohol catalyzed by cation exchange resins: experimental and statistical modeling. 2018 , 125, 535-554		6
705	Gas-to-particle partitioning of major biogenic oxidation products: a study on freshly formed and aged biogenic SOA. 2018 , 18, 12969-12989		6
704	Solubility Prediction Using Neural Network and Chemical Explanation of Deep Learning Model. 2018 , 19, 1-6		O
703	Experimental Isobaric Vapor Liquid Equilibrium for Binary Systems Diethylene Glycol Dibenzoate + Diethylene Glycol, Diethylene Glycol Dibenzoate + Octyl Benzoate, and Ternary System Diethylene Glycol Dibenzoate + Diethylene Glycol + Octyl Benzoate at 1.0152 kPa. <i>Journal of Chemical & Engineering Data</i> , 2018, 63, 3823-3828	2.8	
702	Extension of the F-SAC model to ionic liquids. <i>Fluid Phase Equilibria</i> , 2018 , 477, 87-97	2.5	3
701	Gas-to-particle partitioning of major biogenic oxidation products from monoterpenes and real plant emissions. 2018 ,		1
700	Dependence of Propagation Rate Coefficients in Radical Polymerization on Solution Properties: A Quantitative Thermodynamic Interpretation. 2018 , 12, 1800010		8
699	A model for predicting flash point of alkane-alkane and water-alcohol mixtures by the Cubic-Plus-Association Equation of State. 2018 , 119, 191-197		13
698	Optimization of UNIQUAC interaction parameters for absorption refrigeration machine working fluids. 2018 ,		
697	Method for Estimating Activity Coefficients of Target Components in Poorly Specified Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 7310-7313	3.9	16
696	Isobaric Vapor Liquid Phase Equilibrium Measurements, Correlation, and Prediction for Separation of the Mixtures of Cyclohexanone and Alcohols. <i>Journal of Chemical & Data</i> , 2018, 63, 2038-2045	2.8	4
695	Vapor pressures of diethyl carbonate + ethanol binary mixture and diethyl carbonate + ethanol + isooctane/toluene ternary mixtures at temperatures range of 303.15B23.15 K. 2018 , 264, 32-37		11
694	Experimental study and modeling of citric acid solubility in alcohol mixtures. 2018, 237, 96-102		11
693	Liquid Liquid Equilibria for Ternary (Methyl Propyl Ketone + Hydroquinone or Resorcinol + Water) Systems at 298.15, 318.15, and 333.15 K. <i>Journal of Chemical & Chem</i>	0218	10
692	Phase Equilibria for Systems Containing Refined Soybean Oil plus Cosolvents at Different Temperatures. <i>Journal of Chemical & Engineering Data</i> , 2018 , 63, 1937-1945	2.8	6

691	Development of an inorganic and organic aerosol model (CHIMERE 2017<i>ঝlt;/i> v1.0): seasonal and spatial evaluation over Europe. 2018 , 11, 165-194		32
690	Kinetics, mass transfer, and thermodynamic and statistical modeling study for esterification of valeric acid with n-butanol: Homogeneous and heterogeneous catalysis. 2018 , 50, 710-725		5
689	Hygroscopicity of dimethylaminium-, sulfate-, and ammonium-containing nanoparticles. 2018 , 52, 971-98.	3	3
688	Fully Automated Molecular Design with Atomic Resolution for Desired Thermophysical Properties. Industrial & Samp; Engineering Chemistry Research, 2018, 57, 9683-9692	3.9	3
687	Properties. 2018 , 463-484		
686	Plantwide technoeconomic analysis and separation solvent selection for continuous pharmaceutical manufacturing: Ibuprofen, artemisinin, and diphenhydramine. 2018 , 41, 85-120		O
685	Perspective on PSE in pharmaceutical process development and innovation. 2018, 597-656		5
684	Experimental study of the LL, VL and VLL equilibria of water´+ 1-butanol´+ 2-octanol at 101.3 kPa. Fluid Phase Equilibria, 2018 , 475, 111-117	2.5	2
683	Liquid Liquid Equilibrium for Ternary Systems of 2-Pentanone/Mesityl Oxide + Catechol + Water at 298.2, 318.2, and 333.2 K. <i>Journal of Chemical & Data</i> , 2018, 63, 3117-3124	2.8	9
682	A numerical study of buoyancy-Marangoni convection of volatile binary fluids in confined geometries. 2018 , 127, 308-320		5
681	Experimental Binary VLE Data of Morpholine with 1-Butanol and 3-Methyl-1-butanol Systems. Journal of Chemical & Data, 2018, 63, 3215-3226	2.8	1
680	Design and Analysis of Edible Oil Processes Containing Lipids. 2018, 43, 737-742		1
679	Separation of the Methanoll Mater Mixture Using Ionic Liquid. <i>Industrial & Amp; Engineering Chemistry Research</i> , 2018 , 57, 11167-11177	3.9	20
678	Computer-Aided Molecular Design: Fundamentals, Methods, and Applications. 2018,		14
677	Vaporlliquid Equilibrium of Binary Components of the BrCF2COOCH3\(\mathbb{I}\)F3COOCH3 Quaternary System. <i>Theoretical Foundations of Chemical Engineering</i> , 2018 , 52, 295-306	0.9	1
676	Isobaric vapor-liquid equilibrium, density and speed of sound of binary mixtures 2,2,4-trimethylpentane + 1-butanol or dibutyl ether (DBE) at 101.3 kPa. <i>Fluid Phase Equilibria</i> , 2018 , 2475, 10-17	2.5	7
675	Thermodynamic modeling of asphaltene precipitation in pure and mixed solvents with NRTL-SAC. <i>Fluid Phase Equilibria</i> , 2018 , 473, 255-261	2.5	8
674	Modelling of elemental mercury solubility in natural gas components. 2018 , 233, 558-564		12

673	Generalization of Guggenheim's combinatorial activity coefficient equation. 2018, 266, 467-471	6	· •
672	Phase Equilibrium Involving Xylitol, Water, and Ethylene Glycol or 1,2-Propylene Glycol: Experimental Data, Activity Coefficient Modeling, and Prediction with Artificial Neural 3.9 Network-Molecular Descriptors. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 10675-10683	5	
671	Molecular simulation of volume of mixing, Helmholtz free energy of mixing and entropy of mixing in bulk fluid mixtures. 2018 , 44, 1312-1324	1	-
670	Predicting phase equilibrium for polymer solutions using COSMO-SAC. <i>Fluid Phase Equilibria</i> , 2018 , 472, 75-84	1	ĨO
669	Aerosol sources in the western Mediterranean during summertime: a model-based approach. 2018 , 18, 9631-9659	1	.2
668	A combination of multi-fluid mixture models with COSMO-SAC. <i>Fluid Phase Equilibria</i> , 2018 , 476, 147-1562.5	8	,
667	Prediction of Flash Temperature of Binary Mixtures Containing AlcoholAlcohol and AlcoholAcid Using a Combination of Activity Models and Group Contribution Methods. <i>Journal of Chemical 2.8 & Amp; Engineering Data</i> , 2018 , 63, 3184-3195		
666	Application of COSMO-RS and UNIFAC for ionic liquids based gas separation. 2018 , 192, 816-828	4	ļO
665	Thermodynamic Modeling and Simulation of Natural Gas Dehydration Using Triethylene Glycol with the UMR-PRU Model. <i>Industrial & Engineering Chemistry Research</i> , 2018 , 57, 8584-8604	2	.1
664	Vaporlliquid Equilibria of Binary Systems with Long-Chain Organic Compounds (Fatty Alcohol, Fatty Ester, Acylglycerol, and n-Paraffin) at Subatmospheric Pressures. <i>Journal of Chemical & 2.8 Engineering Data</i> , 2018 , 63, 2840-2847	3	
663	Prediction of the Phase Behavior of Hyperbranched Polymer Solutions by the Group Contribution Method. <i>Theoretical Foundations of Chemical Engineering</i> , 2018 , 52, 447-458	1	-
662	Computer-aided design of optimal environmentally benign solvent-based adhesive products. 2019 , 130, 106518	1	-3
661	Activity Coefficients for Liquid Organic Reactions: Towards a Better Understanding of True Kinetics with the Synthesis of Jasmin Aldehyde as Showcase. 2019 , 20,	5	;
660	Estimation of Structural Parameters of Protic Ionic Liquids for Activity Coefficient Models and Calculations of LLE Phase Diagrams. 2019 , 93, 1312-1316	1	
659	Comparison of the Models for Correlation of Drug Solubility in Ethanol + Water Binary Mixtures. 2019 , 48, 1079-1104	4	
658	110th Anniversary: A Case Study on Developing Accurate and Reliable Excess Gibbs Energy Correlations for Industrial Application. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 12465-372	477 ^C)
657	Release of pharmaceutical cocktails from small polymeric micelles. 2019 , 207, 799-804	3	
656	SolidIliquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry. <i>Journal of Chemical & Differential Scanning Data</i> , 2019 , 64, 5017-5027	4	

655	From graphical to model-based distillation column design: A McCabe-Thiele-inspired mathematical programming approach. <i>AICHE Journal</i> , 2019 , 65, e16731	3.6	9
654	Flash Point of Fatty Acid Methyl Ester Binary Mixtures. <i>Journal of Chemical & Data</i> , 2019, 64, 3465-3472	2.8	7
653	In Silico Prediction of the Thermodynamic Equilibrium of Solute Partition in Multiphase Complex Fluids: A Case Study of Oil-Water Microemulsion. 2019 , 35, 10855-10865		7
652	Machine Learning of Molecular Classification and Quantum Mechanical Calculations. 2019 , 46, 787-792		4
651	An experimental and CFD modeling study of suspended droplets evaporation in buoyancy driven convection. 2019 , 375, 122006		7
650	An Empirical Correlation Relating Equilibrium Compressibility Factors for Pure Substances. 2019 , 40, 1		
649	Ruddlesden P opper 2D Component to Stabilize EsPbI3 Perovskite Phase for Stable and Efficient Photovoltaics. 2019 , 9, 1902529		74
648	Physical modeling of evaporative emission control system in gasoline fueled automobiles: A review. 2019 , 116, 109462		9
647	A predictive group-contribution model for the viscosity of aqueous organic aerosol. 2019,		
646	Predicting solvent effects on relative volatility behavior in extractive distillation using isothermal titration calorimetry (ITC) and molecular modeling (MM). 2019 , 210, 115203		9
645	The UNIFAC-LLE and COSMO-SAC ternary aqueous LLE calculations. <i>Fluid Phase Equilibria</i> , 2019 , 501, 112278	2.5	2
645		2.5	20
	501, 112278 Determination of the Solubility of the Repaglinide Drug in Supercritical Carbon Dioxide: Experimental Data and Thermodynamic Modeling. Journal of Chemical & Data,		
644	Determination of the Solubility of the Repaglinide Drug in Supercritical Carbon Dioxide: Experimental Data and Thermodynamic Modeling. <i>Journal of Chemical & Data</i> , 2019, 64, 5338-5348 Solubility Enhancement of Vitamins in Water in the Presence of Covitamins: Measurements and	2.8	20
644	Determination of the Solubility of the Repaglinide Drug in Supercritical Carbon Dioxide: Experimental Data and Thermodynamic Modeling. <i>Journal of Chemical & Data, 2019, 64, 5338-5348</i> Solubility Enhancement of Vitamins in Water in the Presence of Covitamins: Measurements and ePC-SAFT Predictions. <i>Industrial & Data, 2019, 58, 21761-21771</i> Dispersion activity coefficient models. Part 1: Cubic equations of state. <i>Fluid Phase Equilibria, 2019, 1999</i>	2.8	20
644 643	Determination of the Solubility of the Repaglinide Drug in Supercritical Carbon Dioxide: Experimental Data and Thermodynamic Modeling. <i>Journal of Chemical & Data </i>	2.8	20
644 643 642	Determination of the Solubility of the Repaglinide Drug in Supercritical Carbon Dioxide: Experimental Data and Thermodynamic Modeling. <i>Journal of Chemical & Data</i> , 2019, 64, 5338-5348 Solubility Enhancement of Vitamins in Water in the Presence of Covitamins: Measurements and ePC-SAFT Predictions. <i>Industrial & Dispersion activity coefficient models</i> . Part 1: Cubic equations of state. <i>Fluid Phase Equilibria</i> , 2019, 501, 112275 Physicochemical Properties of Gas. 2019, 13-41	2.8	20 10 2

637	Synthesis and Kinetics of the -(2-Methyl-6-ethyl phenyl)-1-methoxypropyl-2-imine Schiff Base Catalyzed by NKC-9 Cation Exchange Resin. 2019 , 4, 14750-14758	О
636	Modeling solubility of CO gas in room temperature ionic liquids using the COSMOSAC-LANL model: a first principles study. 2019 , 21, 19667-19685	3
635	NUMERICAL AND COMPUTATIONAL ASPECTS OF COSMO-BASED ACTIVITY COEFFICIENT MODELS. 2019 , 36, 587-598	2
634	Analysis of Thermodynamic Models for Simulation and Optimisation of Organic Rankine Cycles. 2019 , 12, 3307	1
633	RH-dependent organic aerosol thermodynamics via an efficient reduced-complexity model. 2019,	1
632	New Predictive Nonrandom Two Liquid Equation for Solidliquid Phase Equilibrium in n-Alkanes Mixture with Multiple Solid Solutions. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 18411-18421	O
631	A new pot still distillation model approach with parameter estimation by multi-objective optimization. 2019 , 130, 106570	5
630	Modeling H2S solubility in aqueous N-methyldiethanolamine solution using a new ePC_SAFT-MB equation of state. <i>Fluid Phase Equilibria</i> , 2019 , 502, 112289	3
629	Isobaric Vapor Diquid Equilibria of Binary Mixtures of Diethyl Carbonate with Isopropyl Acetate, sec-Butyl Acetate, or Isoamyl Acetate at 101.3 kPa. <i>Journal of Chemical & Engineering Data</i> , 2.8 2019 , 64, 5225-5231	3
628	The Generalized Local Composition Model: Its Features and Limitations. 2019 , 93, 1918-1922	
627	Formation and evolution of aqueous organic aerosols via concurrent condensation and chemical aging. 2019 , 265, 45-67	7
626	Solubilities of gases in cycloethers. The solubility of 13 nonpolar gases in 2,5-dimethyltetrahydrofuran at 273.15 to 303.15 K and 101.32 kPa. 2019 , 132, 306-315	3
625	Recent Advances in the Molecular Engineering of Solvents for Reactions. 2019, 17-46	
624	Removal of gaseous acetic acid using ionic liquid [EMIM][BF4]. 2019 , 4, 190-197	21
623	Modeling of Coesterification Process for Biodegradable Poly(Butylene Succinate-co-Butylene Terephthalate) Copolyesters. 2019 , 13, 1800069	3
622	Complexity of Measuring and Representing the Hygroscopicity of Mixed Component Aerosol. 2019 , 123, 1648-1660	12
621	Structural effect on the vapor-liquid equilibrium of toluene-ionic liquid systems. 2019 , 198, 1-15	15
620	Solvent selection for extractive distillation processes to separate close-boiling polar systems. 2019 , 144, 123-134	5

619	Sorption Thermodynamics of COIHD, and CHDH in a Glassy Polyetherimide: A Molecular Perspective. 2019 , 9,		7
618	An Experimental Assessment of Model-Based Solvent Selection for Enhancing Reaction Kinetics. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 13517-13532	3.9	2
617	Hybrid QSPR models for the prediction of the free energy of solvation of organic solute/solvent pairs. 2019 , 21, 13706-13720		19
616	Systematic modeling under uncertainty of single, double and triple effect absorption refrigeration processes. 2019 , 183, 262-278		8
615	Modelling the hygroscopic growth factors of aerosol material containing a large water-soluble organic fraction, collected at the Storm Peak Laboratory. 2019 , 214, 116760		2
614	Nonrandom Two-Liquid Segment Activity Coefficient Model with Association Theory. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 12773-12786	3.9	11
613	110th Anniversary: From Solubility Parameters to Predictive Equation-of-State Modeling. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 12787-12800	3.9	7
612	Modeling the effect of non-ideality, dynamic mass transfer and viscosity on SOA formation in a 3-D air quality model. 2019 , 19, 1241-1261		15
611	Revisiting glycerol esterification with acetic acid over Amberlyst-35 via statistically designed experiments: Overcoming transport limitations. 2019 , 207, 91-104		9
610	Solubility measurements and thermodynamic modeling of pyrazinamide in five different solvent-antisolvent mixtures. <i>Fluid Phase Equilibria</i> , 2019 , 497, 33-54	2.5	7
609	Techno-economic Feasibility of Reactive Distillation for Biodiesel Production from Algal Oil: Comparing with a Conventional Multiunit System. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 12028-12040	3.9	14
608	Investigation of surface tension and surface properties of alkanolamine \blacksquare lcohol mixtures at $T = 313.15$ K and $P = 90.6$ kPa. 2019 , 287, 110924		11
607	Liquid Liquid Equilibrium for Systems Containing Epoxidized Oils, Formic Acid, and Water: Experimental and Modeling. 2019 , 96, 955-965		
606	CAMD for entrainer screening of extractive distillation process based on new thermodynamic criteria. 2019 , 147, 721-733		10
605	Microdroplet nucleation by dissolution of a multicomponent drop in a host liquid. 2019 , 870, 217-246		11
604	NEATIMMR Spectroscopy for the Estimation of Activity Coefficients of Target Components in Poorly Specified Mixtures. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 9155-9165	3.9	9
603	Applications of In Silico Solvent Screening and an Interactive Web-Based Portal for Pharmaceutical Crystallization Process Development. 2019 , 108, 2621-2634		4
602	Partial solvation parameters in conservation science for works of art. 2019 , 39, 1-12		3

601	Geometrical investigation and classification of three-suffix margules binary mixtures including single and double azeotropy. <i>Fluid Phase Equilibria</i> , 2019 , 494, 212-227	2.5	11
600	Absorption refrigeration processes with organic working fluid mixtures- a review. 2019 , 109, 239-270		22
599	CASE STUDIES ON THE USE OF DISTILLATION IN THE PHARMACEUTICAL INDUSTRY. 2019 , 787-797		1
598	Activity-based analysis of potentiometric pH titrations. 2019 , 1075, 49-56		1
597	Liquid-liquid equilibrium study for ternary systems of water + propargyl alcohol + solvents at 308.2 K: Measurement and thermodynamic modelling. 2019 , 135, 149-154		5
596	Model Performances Evaluated for Infinite Dilution Activity Coefficients Prediction at 298.15 K. <i>Industrial & Engineering Chemistry Research</i> , 2019 ,	3.9	11
595	Eco-efficient recovery of bio-based volatile C2-6 fatty acids. 2019 , 12, 92		25
594	Application of the group contribution volume translated Peng R obinson equation of state to new commercial refrigerant mixtures. 2019 , 103, 316-328		6
593	Prediction of the melting behavior of edible fats using UNIFAC and UNIQUAC models. <i>Fluid Phase Equilibria</i> , 2019 , 493, 58-66	2.5	6
592	Modelling and experimental validation of dimethyl carbonate solvent recovery from an aroma mixture by batch distillation. 2019 , 147, 1-17		1
591	Toward Thermodynamic Predictions of Aqueous Vitamin Solubility: An Activity Coefficient-Based Approach. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 7362-7369	3.9	31
590	Vapor-liquid (azeotropic systems) and liquid-liquid equilibrium calculations using UNIFAC and NRTL-SAC activity coefficient models. <i>Fluid Phase Equilibria</i> , 2019 , 494, 33-44	2.5	4
589	Computer-aided reaction solvent design based on transition state theory and COSMO-SAC. 2019 , 202, 300-317		23
588	Production of Oxymethylene Dimethyl Ethers from Hydrogen and Carbon Dioxide P art I: Modeling and Analysis for OME1. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 4881-4889	3.9	29
587	Capturing volatile ester compounds from gas mixture with ionic liquids. 2019 , 281, 517-527		8
586	Studies for removal of tar from producer gas in small scale biomass gasifiers using biodiesel. 2019 , 123, 123-133		12
585	Molecular design of solvents for CO2 capture using a group contribution EOS. <i>Fluid Phase Equilibria</i> , 2019 , 490, 114-122	2.5	4
584	General Procedure for Process Simulation. 2019 , 15-59		

583	Phase Equilibrium Involving Xylose, Water, and Ethylene Glycol or 1,2-Propylene Glycol at Different Temperatures. <i>Journal of Chemical & Engineering Data</i> , 2019 , 64, 2163-2169	2.8	1
582	SOLVENTS USE IN VARIOUS INDUSTRIES. 2019 , 901-1124		1
581	Molecular simulations of enzymes under non-natural conditions. 2019 , 227, 1631-1638		1
580	Liquid Phase Density, Sound Speed, and Vapor Pressure of Linear Alkanes Using the Mattedillavares Lastier Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 6767-6777	3.9	2
579	Modelling of hydrogen vapor-liquid equilibrium with oil & gas components. <i>Fluid Phase Equilibria</i> , 2019 , 494, 125-134	2.5	4
578	A Group Contribution Equation of State for Biorefineries. GCA-EOS Extension to Bioether Fuels and Their Mixtures with n-Alkanes. <i>Journal of Chemical & Data</i> , 2019, 64, 2170-2185	2.8	O
577	Multi-component droplet evaporation model incorporating the effects of non-ideality and thermal radiation. 2019 , 136, 962-971		12
576	Production of Oxymethylene Dimethyl Ethers from Hydrogen and Carbon DioxidePart II: Modeling and Analysis for OME3B. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 5567-557	′8 ^{3.9}	25
575	Modeling of solid-liquid equilibrium using a modified group contribution based NRTL model. <i>Fluid Phase Equilibria</i> , 2019 , 492, 118-136	2.5	4
574	Prediction of Flash-Point Temperature of Alcohol/Biodiesel/Diesel Fuel Blends. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 6860-6869	3.9	19
573	Simulation Study on the Influence of Gas Mole Fraction and Aqueous Activity under Phase Equilibrium. 2019 , 7, 58		1
572	Solubility Prediction of Different Forms of Pharmaceuticals in Single and Mixed Solvents Using Symmetric Electrolyte Nonrandom Two-Liquid Segment Activity Coefficient Model. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 4267-4276	3.9	5
571	Can we safely predict solvation Gibbs energies of pure and mixed solutes with a cubic equation of state?. 2019 , 91, 1295-1307		3
570	Modeling Equilibrium Behavior of Nylon 6, Nylon 6,6 and Nylon 6/6,6 Copolymer. 2019 , 13, 1800078		2
569	Molecular simulation as a computational pharmaceutics tool to predict drug solubility, solubilization processes and partitioning. 2019 , 137, 46-55		42
568	Implementation of a Property Database and Thermodynamic Calculations in OpenModelica for Chemical Process Simulation. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 7551-7560	3.9	3
567	Thermodynamic Activity-Based Michaelis Constants. 2019,		2
566	Thermodynamic models applied to CO2 absorption modelling. 2019 ,		4

565	Relative-humidity-dependent organic aerosol thermodynamics via an efficient reduced-complexity model. 2019 , 19, 13383-13407		10
564	Design of Extractive Reaction Systems. 2019 , 91, 1766-1776		3
563	The Acidity of Atmospheric Particles and Clouds. 2019,		8
562	Estimation of the Emission Characteristics of SVOCs from Household Articles Using Group Contribution Methods. 2020 , 54, 110-119		8
561	Optimal Design of Experiments for Liquid Liquid Equilibria Characterization via Semidefinite Programming. 2019 , 7, 834		1
560	Solvent screening and liquid-liquid measurement for extraction of phenols from aromatic hydrocarbon mixtures. 2019 , 129, 12-21		29
559	Design and economic evaluation of energy-saving industrial distillation processes for separating close-boiling cyclohexanone-cyclohexanol mixture. 2019 , 211, 279-289		12
558	Process modelling, design and technoeconomic Liquidliquid Extraction (LLE) optimisation for comparative evaluation of batch vs. continuous pharmaceutical manufacturing of atropine. 2019 , 124, 28-42		5
557	Novel phase diagrams of aqueous two-phase systems based on 1,4-bis-(2-hydroxypropyl)-piperazine + Na2CO3 + H2O: Equilibrium data and correlation. <i>Fluid Phase Equilibria</i> , 2019 , 485, 128-134	2.5	
556	Hansen solubility parameters and thermodynamic modeling for LLE description during glycerol-settling in ester production from coconut oil. 2019 , 241, 725-732		O
555	Modeling and analysis of new reactor concepts for poly(ethylene terephthalate) esterification process. 2019 , 135, 217-226		
554	An evaluation of in-silico methods for predicting solute partition in multiphase complex fluids A case study of octanol/water partition coefficient. 2019 , 197, 150-158		14
553	On the mixing rules matter: The VLE predictions for binary systems. <i>Fluid Phase Equilibria</i> , 2019 , 484, 1-14	2.5	1
552	Separation of heterocyclic nitrogen compounds from coal tar fractions via ionic liquids: COSMO-SAC screening and experimental study. 2019 , 206, 1199-1217		21
551	Development of a Model for Electrostatic Contribution to the Osmotic Coefficient of Aqueous Electrolytes. <i>Industrial & Development of Electrolytes</i> .	3.9	1
550	Solubility and critical surface in the system propionic acid@thanol@thyl propionateWater at 293.15, 303.15 and 313.15 K. 2019 , 132, 113-121		12
549	OptCAMD: An optimization-based framework and tool for molecular and mixture product design. 2019 , 124, 285-301		40
548	Design of bio-oil additives via computer-aided molecular design tools and phase stability analysis on final blends. 2019 , 123, 257-271		13

547	Chemical reaction between sodium pyruvate and ammonium sulfate in aerosol particles and resultant sodium sulfate efflorescence. 2019 , 215, 554-562		11
546	Classical Models Part 2: Activity Coefficient Models and Applications. 2019 , 103-162		
545	Liquid[liquid and Vapor[liquid[liquid Equilibrium in Food Processes. 2019 , 275-334		
544	Equilibrium in Pressurized Systems (Sub and Supercritical). 2019 , 385-418		1
543	Liquid-liquid equilibria and density data for pseudoternary systems of refined soybean oil + (hexanal, or heptanal, or butyric acid, or valeric acid, or caproic acid, or caprylic acid) + dimethyl sulfoxide at 298.15 K. 2019 , 131, 149-158		5
542	Prediction of Mefenamic Acid Solubility and Molecular Interaction Energies in Different Classes of Organic Solvents and Water. <i>Industrial & Engineering Chemistry Research</i> , 2019 , 58, 762-770	3.9	9
541	Vapor liquid equilibrium prediction of methanolibnic liquid systems using UNIFAC model to select alternative working fluids of absorption cycle. 2019 , 14, e2281		4
540	Improving the Predictability of Chemical Equilibrium Software. <i>Industrial & Discourse Engineering Chemistry Research</i> , 2019 , 58, 411-419	3.9	3
539	Microscopic mechanism of the interaction between water and formic acid-sodium chloride aerosol. 2019 , 344, 46-57		3
538	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
537	Predicting solid-liquid-vapor equilibria in highly asymmetric paraffinic systems with EOS-GE model. <i>Fluid Phase Equilibria</i> , 2019 , 480, 1-10	2.5	2
536	Modeling Reactive Mixtures: Case Study for Spills of Formaldehyde Solutions. 2019 , 38, 61-70		
535	Measurements and thermodynamic modelling of liquid II quid equilibrium of PEG 6000 phosphate affinity aqueous two-phase systems at various ligand concentrations and pH. 2020 , 58, 483-499		
534	Investigation of liquidIlquid equilibrium of the ternary system (water + 1,6-diaminohexane + 2-methyl-1-propanol or 3-methyl-1-butanol) at different temperatures. 2020 , 28, 191-197		4
533	Carrier-Fluid Screening for a Three-Phase Sublimation Refrigeration Cycle with CO2 Using Reference Equations of State and COSMO-SAC. <i>Journal of Chemical & Data</i> , 2020, 65, 1124-1134	2.8	2
532	Design and optimization of an acetic acid recovery system via extraction distillation using an isopropyl acetate + isopropanol mixed solvent. 2020 , 207, 1625-1635		1
531	Thermodynamic and Transport Properties Modeling of Deep Eutectic Solvents: A Review on gE-Models, Equations of State, and Molecular Dynamics. <i>Journal of Chemical & Data</i> , 2020 , 65, 943-967	2.8	24
530	Process design and techno-economic analysis of gas and aqueous phase maleic anhydride production from biomass-derived furfural. 2020 , 10, 1021-1033		13

529	Extended Pitzer D ebyell dkel Model for Long-Range Interactions in Ionic Liquids. <i>Journal of Chemical & Data</i> , 2020 , 65, 1019-1027	2.8	8
528	Isobaric Vapor Liquid Equilibrium Determination for 1,3,5-Trimethylbenzene + Ethanol and 1,3,5-Trimethylbenzene + n-Butanol Binary Systems. 2020 , 64, 446-456		
527	Inverse-QSPR for de novo Design: A Review. 2020 , 39, e1900087		17
526	Extending the UNIFAC model for ionic liquid lolute systems by combining experimental and computational databases. <i>AICHE Journal</i> , 2020 , 66, e16821	3.6	29
525	Predicting wax appearance temperature and precipitation profile of normal alkane systems: An explicit co-crystal model. <i>Fluid Phase Equilibria</i> , 2020 , 509, 112466	2.5	2
524	Flash point of binary mixtures of chlorinated hydrocarbons with toluene and their predictability with existing mixing rule. 2020 , 39, e12127		1
523	A predictive power sequence equation for vapor pressures of pure organic fluids and partial pressures in multicomponent systems in equilibrium. <i>Fluid Phase Equilibria</i> , 2020 , 506, 112409	2.5	1
522	Predictive models for physical properties of fats, oils, and biodiesel fuels. <i>Fluid Phase Equilibria</i> , 2020 , 508, 112440	2.5	13
521	A model-based solvent selection and design framework for organic coating formulations. 2020 , 140, 105471		5
520	Prediction of solid solute solubility in supercritical carbon dioxide with and without organic cosolvents from PSRK EOS. 2020 , 158, 104735		8
519	The role of physicochemical properties in the nanoprecipitation of cellulose acetate. 2020 , 230, 115628	3	4
518	Study of FAME model systems: Database and evaluation of predicting models for biodiesel physical properties. 2020 , 151, 837-845		2
517	Transesterification of triolein and methanol with Novozym 435 using co-solvents. 2020 , 263, 116600		4
516	Implementation of the UNIQUAC model in the OpenCalphad software. <i>Fluid Phase Equilibria</i> , 2020 , 507, 112398	2.5	3
515	Simple solvatochromic spectroscopic quantification of long-chain fatty acids for biological toxicity assay in biogas plants. 2020 , 27, 17596-17606		1
514	Density-based UNIFAC model for solubility prediction of solid solutes in supercritical fluids. <i>Fluid Phase Equilibria</i> , 2020 , 506, 112376	2.5	1
513	The prediction multi-phase, multi reactant equilibria by minimizing the Gibbs energy of the system: Review of available techniques and proposal of a new method based on a Monte Carlo technique. 2020 , 216, 115433		7
512	Vapor [lquid and chemical equilibria model for formaldehyde´+ 1,3,5-trioxane´+ methanol´+ salt´+ water system. <i>Fluid Phase Equilibria</i> , 2020 , 507, 112434	2.5	4

511	Modeling of precipitation considering multi-component form of Asphaltene using a solid solution framework. 2020 , 263, 116766		4
510	Computer-aided solvent selection and design for efficient chemical processes. 2020 , 27, 35-44		29
509	Water sorption thermodynamics in glassy polymers endowed with hydrogen bonding interactions. 2020 , 63, 1		2
508	Prediction of liquid-liquid equilibria of multicomponent fatty systems using the ASOG method. <i>Fluid Phase Equilibria</i> , 2020 , 506, 112400	2.5	1
507	Predicting phase equilibrium of aqueous sugar solutions and industrial juices using COSMO-SAC. 2020 , 274, 109836		8
506	A Discrete Modeling Approach for Excess Gibbs-energy Models Combined with Molecular Sampling. 2020 , 48, 169-174		
505	Computer-aided Solvent Mixture Design for the Crystallisation and Isolation of Mefenamic Acid. 2020 , 48, 649-654		1
504	Comparison of kriging, machine learning algorithms and classical thermodynamics for correlating the formation conditions for CO2 gas hydrates and semi-clathrates. 2020 , 84, 103659		4
503	Investigating Various Parametrization Strategies for Pharmaceuticals within the PC-SAFT Equation of State. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 5753-5767	2.8	6
502	Flash point prediction with UNIFAC type models of ethylic biodiesel and binary/ternary mixtures of FAEEs. 2020 , 281, 118717		9
501	Organic Solvent Forward Osmosis of Graphene Oxide-Based Membranes for Enrichment of Target Products. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 19012-19019	3.9	3
500	Scalable Steam Additives for Enhancing In-Situ Bitumen Recovery in SAGD Process. 2020 ,		
499	Liquid Diquid Equilibria for the Quaternary System: Diisopropyl Ether + n-Pentanol + Phenol + Water at 298.15 K. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 5210-5217	2.8	1
498	Solubility Behaviors and Correlations of Common SolventAntisolvent Systems. 2020 , 24, 2722-2727		1
497	Prediction of Phase Behavior of CO2 Absorbents Using Conductor-like Screening Model for Real Solvents (COSMO-RS): An Approach to Identify Phase Separation Solvents of Amine/Ether/Water Systems upon CO2 Absorption. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 19020-19029	3.9	4
496	A new computational method for molecular design of a liquid liquid extractant and related phase equilibrium based on group contribution. 2020 , 5, 1524-1537		
495	Comparative analysis of phase diagrams of organochlorosilane/organoalkoxysilaneBolventDvater systems. 2020 , 69, 1061-1071		О
494	Removal of Methyl Ethyl Ketone and Sec-Butanol from Hydrogen by Absorption with Ionic Liquids. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 14476-14484	3.9	2

493	Effect of chemical aging of aqueous organic aerosols on the rate of their steady-state nucleation. 2020 , 22, 17612-17619		2
492	Integration of modern computational chemistry and ASPEN PLUS for chemical process design. <i>AICHE Journal</i> , 2020 , 66, e16987	3.6	3
491	Impacts of water partitioning and polarity of organic compounds on secondary organic aerosol over eastern China. 2020 , 20, 7291-7306		5
490	References. 2020 , 331-346		
489	SEPP: Segment-Based Equation of State Parameter Prediction. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 5830-5843	2.8	2
488	Machine learning with physicochemical relationships: solubility prediction in organic solvents and water. 2020 , 11, 5753		32
487	Methodology to Predict Thermodynamic Data from Spectroscopic Analysis. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 21548-21566	3.9	2
486	Expanding the Applications of the SAFT-Mie Group-Contribution Equation of State: Prediction of Thermodynamic Properties and Phase Behavior of Mixtures. <i>Journal of Chemical & Data</i> , 2020, 65, 5862-5890	2.8	10
485	Chemoinformatics for the Safety of Energetic and Reactive Materials at Ineris. 2020,		0
484	Phase Equilibria of Ternary Liquidliquid Systems (Water + C1\(\mathbb{I}\)4 Monocarboxylic Acids + Dibutyl Ether) at Three Different Temperatures: Modeling with A-UNIFAC. 2020 , 49, 1009-1028		1
483	Experimental methods in chemical engineering: Process simulation. 2020 , 98, 2301-2320		6
482	Crystalline Multicomponent Solids: An Alternative for Addressing the Hygroscopicity Issue in Pharmaceutical Materials. 2020 , 20, 6245-6265		26
481	Prediction of thermodynamic properties of organic mixtures: Combining molecular simulations with classical thermodynamics. <i>Fluid Phase Equilibria</i> , 2020 , 523, 112759	2.5	3
480	Evaluating the direct CO2 to diethyl carbonate (DEC) process: Rigorous simulation, techno-economical and environmental evaluation. 2020 , 41, 101254		10
479	Measurement and prediction of thermophysical properties of binary mixtures of dicyclopentadiene with methylcyclohexane, toluene, and p-xylene. 2020 , 685, 178536		4
478	. 2020,		3
477	Ordered Hydrogen-Bonded Alcohol Networks Confined in Lewis Acid Zeolites Accelerate Transfer Hydrogenation Turnover Rates. 2020 , 142, 19379-19392		22
476	Thermodynamic gE Models and Equations of State for Electrolytes in a Water-Poor Medium: A Review. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 5073-5082	2.8	8

Contaminate removal with nanoporous carbon modeling and simulation. **2020**, 305-323

474	Application of ePC_SAFT-MB EoS in prediction of VLE for CO2+MDEA+H2O ternary and H2O+MDEA+CO2-CH4 quaternary mixtures. <i>Fluid Phase Equilibria</i> , 2020 , 525, 112801	2.5	1
473	Active learning-driven quantitative synthesis tructure property relations for improving performance and revealing active sites of nitrogen-doped carbon for the hydrogen evolution reaction. 2020 , 5, 2134-2147		8
472	Liquid Diquid Equilibrium and Data Correlation for Quaternary (Methyl Isobutyl Ketone + n-Pentanol + Phenol + Water) System at 101 kPa and 298.2 K: Phenol Coextraction with Synergistic Solvents. Journal of Chemical & Engineering Data, 2020, 65, 4567-4574	2.8	3
471	Hybridizing physical and data-driven prediction methods for physicochemical properties. 2020 , 56, 124	407-124	410
470	Gas Solubility in Ionic Liquids: UNIFAC-IL Model Extension. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 16805-16821	3.9	11
469	Highly efficient, low-temperature hydrogen release from perhydro-benzyltoluene using reactive distillation. 2020 , 13, 3119-3128		14
468	Multiscale Simulation of Vinyl Acetate Systems Applied in the Industrial Gas Separation Column. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 20428-20436	3.9	
467	Binary mixtures of semicrystalline polymers with low-molecular-mass compounds: thermal behaviour and phase structure. 2020 , 89, 311-338		3
466	Perspectives on the Current State, Challenges, and Opportunities in Pharmaceutical Crystallization Process Development. 2020 , 20, 7568-7581		25
465	Cluster-Based Thermodynamics of Interacting Dice in a Lattice. 2020 , 22,		
464	Coupled Simulation of a Vacuum Creation System and a Rectification Column Block. 2020 , 8, 1333		3
463	Geometric investigation of the three-coefficient Redlich-Kister expansion global phase diagram for binary mixtures. <i>Fluid Phase Equilibria</i> , 2020 , 525, 112728	2.5	2
462	Vapor I liquid 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 & Data</i> , 2020 , 65, 2405-2421	2.8	7
461	Modeling organic aerosol over Europe in summer conditions with the VBS-GECKO parameterization: sensitivity to secondary organic compound properties and IVOC (intermediate-volatility organic compound) emissions. 2020 , 20, 4905-4931		3
460	Determination and correlation of temperature and pH value dependent solubility of dl-methionine. <i>AICHE Journal</i> , 2020 , 66, e16270	3.6	3
459	The Acidity of Atmospheric Particles and Clouds. 2020 , 20, 4809-4888		165
458	Modeling the Physicochemical Properties of Natural Deep Eutectic Solvents. 2020 , 13, 3789		30

457	UNIFAC Model for Ionic Liquids. 2. Revision and Extension. <i>Industrial & Extension amp; Engineering Chemistry Research</i> , 2020 , 59, 10172-10184	12
456	Separation of isopropyl alcohol and isopropyl ether with ionic liquids as extractant based on quantum chemical calculation and liquid-liquid equilibrium experiment. 2020 , 247, 116937	23
455	Modeling vapour-liquid phase equilibrium for the aqueous solutions of formaldehyde and electrolyte. 2020 , 150, 106181	O
454	A predictive group-contribution model for the viscosity of aqueous organic aerosol. 2020 , 20, 2987-3008	17
453	Prediction of CO2 solubility in ionic liquids using machine learning methods. 2020 , 223, 115752	55
452	Isothermal measurement and modeling of VLE properties for 2,3,3,3-tetrafluoroprop-1-ene + trifluoromethane + tetrafluoromethane ternary system at temperatures from 253.15 K to 273.15 K. 2020 , 117, 284-294	1
451	tert-ButanolWater mixture separation by extractive distillation: Application of experimental data in process simulations. 2020 , 251, 116968	7
450	Solubility, similarity, and compatibility: A general-purpose theory for the formulator. 2020 , 48, 65-76	8
449	Experimental and modelling study of the phase behavior of (methyl propanoate + carbon dioxide) at temperatures between (298.15 and 423.15) K and pressures up to 20 MPa. Fluid Phase Equilibria, 2.5 2020 , 519, 112653	1
448	Aggregation thermodynamics of asphaltenes: Prediction of asphaltene precipitation in petroleum fluids with NRTL-SAC. <i>Fluid Phase Equilibria</i> , 2020 , 520, 112655	3
447	Correlation and prediction of small to large sized pharmaceuticals solubility, and crystallization in binary and ternary mixed solvents using the UNIQUAC-SAC model. <i>Fluid Phase Equilibria</i> , 2020 , 519, 112656	5
446	Isobaric Vaporlliquid Equilibria at 50.0, 101.3, and 200.0 kPa. Density and Speed of Sound at 101.3 kPa and 298.15 K of Binary Mixtures HFE-7100 + 2-Propanol. <i>Journal of Chemical & Data</i> , 2020, 65, 4290-4298	O
445	Esterification using a liquid lipase to remove residual free fatty acids in biodiesel. 2020 , 97, 213-221	9
444	Simplified COSMO-SAC-based phase equilibria predictions for extractive distillation of toluenefleptane mixtures using ionic liquids. 2020 , 15, e2513	7
443	Flash point and excess molar volumes of binary mixtures containing d-limonene and alcohol compounds from propanol to dodecanol. 2020 , 150, 106224	1
442	Hygroscopicity of amino acids and their effect on the water uptake of ammonium sulfate in the mixed aerosol particles. 2020 , 734, 139318	8
441	Generic Context-Aware Group Contributions. 2020 , PP,	
440	Influence of non-ideal behavior on esterification kinetics modeling. 2020 , 130, 617-632	1

439	An extended COSMO-SAC method for the prediction of carboxylic acid solubility. <i>Fluid Phase Equilibria</i> , 2020 , 521, 112673	4
438	SSH-Aerosol v1.1: A Modular Box Model to Simulate the Evolution of Primary and Secondary Aerosols. 2020 , 11, 525	6
437	Assessment of the SM12, SM8, and SMD Solvation Models for Predicting Limiting Activity Coefficients at 298.15 K. 2020 , 8, 623	6
436	Design of Solvent Mixtures for Selective Extraction by Quantifying Thermodynamic and Sustainability Aspects. 2020 , 4, 297-308	1
435	Towards a predictive thermodynamic description of sorption processes in polymers: The synergy between theoretical EoS models and vibrational spectroscopy. 2020 , 140, 100525	17
434	Predictive models for the phase behaviour and solution properties of weak electrolytes: nitric, sulphuric, and carbonic acids. 2020 , 22, 15248-15269	7
433	Phase equilibria of binary and ternary polymer solutions using modified UNIQUAC-based local composition model. 2020 , 142, 1493-1510	1
432	Experimental Data on Chemical Equilibrium in the System with Ethyl Formate Synthesis Reaction at 298.15 K. <i>Journal of Chemical & Engineering Data</i> , 2020 , 65, 2578-2582	2
431	Evaluation of a Variation of the Differential Scanning Calorimetry Technique for Measuring Boiling Points of Binary Mixtures at Subatmospheric Pressures. <i>Journal of Chemical & Engineering Data</i> , 2.8, 2020, 65, 3334-3343	2
430	Bibliography. 2020 , 431-442	
429	Kinetic study on the reaction of palmitic acid with ethanol catalyzed by deep eutectic solvent based on dodecyl trimethyl ammonium chloride. 2020 , 37, 1482-1489	5
428	Deep learning and knowledge-based methods for computer-aided molecular design E oward a unified approach: State-of-the-art and future directions. 2020 , 141, 107005	35
427	Property Data Estimation for Hemiformals, Methylene Glycols and Polyoxymethylene Dimethyl Ethers and Process Optimization in Formaldehyde Synthesis. 2020 , 13, 3401	4
426	Intensification of 2-Methyl-1,3-Dioxolane hydrolysis for recovery of ethylene glycol through reactive distillation: Kinetics and process design. 2020 , 154, 108012	4
425	Combined Experimental and Theoretical Studies on the Prediction of the Isobaric Vaporlliquid Association Phenomena for Binary and Ternary Mixtures of Water, Ethanoic Acid, and Propanoic Acid. Industrial & Engineering Chemistry Research, 2020, 59, 13290-13304	2
424	Systematic Green Solvent Selection for the Hydroformylation of Long-Chain Alkenes. 2020,	2
423	Sugar replacement with zwitterionic plasticizers like amino acids. <i>Food Hydrocolloids</i> , 2020 , 109, 106113 10.0	5 8

421	Modeling and Simulation of Single Ethanol/Water Droplet Evaporation in Dry and Humid Air. 2020 , 192, 1233-1252		9
420	Thermodynamic and ecological preselection of synthetic fuel intermediates from biogas at farm sites. 2020 , 10,		7
419	Vapor Liquid Equilibria of the Ionic Liquid 1-Hexyl-3-methylimidazolium Triflate (C6mimTfO) with n-Alkyl Alcohols. <i>Industrial & amp; Engineering Chemistry Research</i> , 2020 , 59, 5142-5157	3.9	2
418	Expanding the Solubility Parameter Method MOSCED to Pyridinium-, Quinolinium-, Pyrrolidinium-, Piperidinium-, Bicyclic-, Morpholinium-, Ammonium-, Phosphonium-, and Sulfonium-Based Ionic Liquids. 2020 , 5, 3863-3877		7
417	Synergistic Extraction of Hydroquinone from an Aqueous Solution with a Solvent Mixture of Diisopropyl Ether and n-Pentanol at T = 298.15 K and P = 101.3 kPa: Liquidliquid Equilibria and Data Correlation. <i>Journal of Chemical & Data</i> (2020, 65, 1538-1546)	2.8	1
416	An approach for simultaneous computer-aided molecular design with holistic sustainability assessment: Application to phase-change CO2 capture solvents. 2020 , 135, 106769		20
415	Toward Rational Functionalization of Ionic Liquids for Enhanced Extractive Desulfurization: Computer-Aided Solvent Design and Molecular Dynamics Simulation. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 2093-2103	3.9	14
414	Benzene-Induced Crystallization of PPO: A Combined Thermodynamic and Vibrational Spectroscopy Study. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 5402-5411	3.9	8
413	Machine Learning in Thermodynamics: Prediction of Activity Coefficients by Matrix Completion. 2020 , 11, 981-985		17
412	Fundamental Thermodynamic Models for Mixtures Containing Ammonia. <i>Fluid Phase Equilibria</i> , 2020 , 511, 112496	2.5	3
411	Formation of polyethersulfone membranes via nonsolvent induced phase separation process from dissipative particle dynamics simulations. 2020 , 599, 117826		16
410	Improved Prediction of Phase Behaviors of Ionic Liquid Solutions with the Consideration of Directional Hydrogen Bonding Interactions. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 3550-3559	3.9	2
409	The use of process simulation in supercritical fluids applications. 2020 , 5, 424-451		17
408	Ionic-Liquid-Based Bioisoprene Recovery Process Design. <i>Industrial & amp; Engineering Chemistry Research</i> , 2020 , 59, 7355-7366	3.9	5
407	Prediction of the Distillation Curve and Vapor Pressure of Alcohol@asoline Blends Using Pseudocomponents and an Equation of State. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 8361-8373	3.9	5
406	Renormalization Group Approach to Binary Liquid Liquid Equilibria. <i>Industrial & amp; Engineering Chemistry Research</i> , 2020 , 59, 9611-9618	3.9	2
405	Expanding SAFT-Miel Application to Dipolar Species: 2-Ketones, 3-Ketones, and Propanoate Esters. <i>Industrial & Esters & Industrial & In</i>	3.9	1
404	Conventional and advanced exergy analysis of an air-cooled type of absorption-ejection refrigeration cycle with R290-mineral oil as the working pair. 2020 , 210, 112703		8

403	Comparison of MOSCED (NRTL) model results with regular correlative and predictive models based on vapor-liquid equilibrium calculations for azeotropic systems. <i>Fluid Phase Equilibria</i> , 2020 , 516, 112592 ^{2.5}	
402	Modeling of Simultaneous Chemical and Phase Equilibria in Systems Involving Non-reactive and Reactive Azeotropes. <i>Industrial & amp; Engineering Chemistry Research</i> , 2020 , 59, 8836-8847	2
401	Experimental Binary Vapor Liquid Equilibrium Data of Morpholine with Methanol, 1-Propanol, and 2-Ethoxyethanol. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 178-188	1
400	Thermodynamic modeling and rational design of ionic liquids for pre-combustion carbon capture. 2021 , 229, 116076	29
399	Structural effects on thermodynamic behavior and hydrogen bond interactions of waterIbnic liquid systems. 2021 , 230, 116186	8
398	ASTM D86 distillation curve: Experimental analysis and premises for literature modeling. 2021 , 284, 118958	O
397	Intelligent modelling and analysis of biodiesel/alcohol/glycerol liquid-liquid equilibria. 2021, 322, 114972	3
396	Interface-resolved simulation of the evaporation and combustion of a fuel droplet suspended in normal gravity. 2021 , 287, 119413	3
395	Synergistic Computational Modeling Approaches as Team Players in the Game of Solubility Predictions. 2021 , 110, 22-34	2
394	Evaluating ignition propensity of high cycloparaffinic content alternative jet fuel by a chemical functional group approach. 2021 , 223, 243-253	4
393	Experimental results for the vapor liquid equilibria of (formaldehyde '+ '1,3,5-trioxane '+ 'methanol '+ 'salt '+ 'water) systems and comparison with predictions. 2021 , 32, 291-300	1
392	Comparison of thermal and chemical enhanced recovery of DNAPL in saturated porous media: 2D tank pumping experiments and two-phase flow modelling. 2021 , 760, 143958	6
391	Reaction kinetic studies on the immobilized-lipase catalyzed enzymatic resolution of 1-phenylethanol transesterification with ethyl butyrate. 2021 , 39, 29-40	2
390	Investigating the use of excess Gibbs energy to predict the hydrophobicity of a mineral treated with a collector. 2021 , 160, 106692	2
389	Towards a universal digital chemical space for pure component properties prediction. <i>Fluid Phase Equilibria</i> , 2021 , 527, 112829	1
388	Predictive molecular thermodynamic models for ionic liquids. 2021 , 209-241	
387	Production of nutraceutical astaxanthin from waste resources. 2021 , 181-205	O
386	Neural recommender system for the activity coefficient prediction and UNIFAC model extension of ionic liquid-solute systems. <i>AICHE Journal</i> , 2021 , 67, e17171	14

385	A global transform for the general formulation of liquid viscosities with significant linearizing benefits: a case study on ionic liquid mixtures. 2021 , 23, 22551-22566	-	1
384	Cellobiose as a Model Carbohydrate for Predicting Solubilities in Nonaqueous Solvents. <i>Industrial & Solubilities in Monaqueous Solvents</i> . <i>Industrial 3.9</i>		2
383	Role of Computational Variables on the Performances of COSMO-SAC Model: A Combined Theoretical and Experimental Investigation. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 3.9 60, 2314-2325	1	
382	References. 2021 , 177-183		
381	Application of Dimethyl Carbonate Assisted Chemical Looping Technology in the Separation of the Ethylene Glycol and 1,2-Butanediol Mixture and Coproduction of 1,2-Butene Carbonate. <i>Industrial & Amp; Engineering Chemistry Research</i> , 2021 , 60, 2249-2264	:	2
380	Excess mixture properties and activity coefficients. 2021 , 281-364		1
379	UNIFAC y∏ lītemi kullan l arak etilasetat-etanol sistemi i∏ līh izotermal buhar-s ṽ dengesi kestirimi.		
378	Liquid-liquid equilibrium and tie-line data for systems of water + acetic acid + organic solvents (chloroform, dichloromethane, and cyclohexane). 2021 ,		
377	Prediction of Excess Enthalpy Using Volume-Translated PengRobinson Equation of State. 2021, 5, 8		
376	Organosulfates from Dark Aqueous Reactions of Isoprene-Derived Epoxydiols Under Cloud and Fog Conditions: Kinetics, Mechanism, and Effect of Reaction Environment on Regioselectivity of Sulfate Addition. 2021 , 5, 474-486		4
375	Energy-efficient recovery process of 2,3-butanediol using 2-heptanol extraction. 2021 , 160, 108286	-	9
374	An approach to low-temperature flame spray pyrolysis for the synthesis of temperature-sensitive materials: Application to Li1.2Mn0.54Ni0.13Co0.13O2. 2021 , 5, 100020	2	2
373	Automated robotic platforms in design and development of formulations. AICHE Journal, 2021, 67, e17248		4
372	Physicochemical Characterization and Simulation of the Solid-Liquid Equilibrium Phase Diagram of Terpene-Based Eutectic Solvent Systems. 2021 , 26,	;	7
371	Total vapor pressure of hydrophobic deep eutectic solvents: Experiments and modelling. 2021 , 325, 11522	7	9
370	Simulating combustion of a seven-component surrogate for a gasoline/ethanol blend including soot formation and comparison with experiments. 2021 , 288, 119451		6
369	Isobaric Vaporlliquid Equilibria for Binary Mixtures of 2-Phenylethanol with 1-Phenylethanol, 2-Phenylpropan-2-ol, Ethylbenzene, and Isopropylbenzene at 101.3 kPa. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 1754-1762	:	2
368	Computer-Aided Ionic Liquid Design and Experimental Validation for Benzeneffyclohexane Separation. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 4951-4961	:	2

367	Dispersions of Zirconia Nanoparticles Close to the Phase Boundary of Surfactant-Free Ternary Mixtures. 2021 , 37, 4072-4081		2
366	Dependence of Copolymer Composition in Radical Polymerization on Solution Properties: a Quantitative Thermodynamic Interpretation. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 10566-10583	3.9	1
365	The Effect of Droplet Temperature Model Choice on Gasoline Droplet and Spray Simulation.		
364	Thermodynamic Modeling of Salting Effects in Solvent Extraction of Cobalt(II) from Chloride Media by the Basic Extractant Methyltrioctylammonium Chloride. 2021 , 6, 11355-11366		4
363	Phase equilibria modeling of biorefinery-related systems: a systematic review. 2021,		
362	Predicting evaporation dynamics of a multicomponent gasoline/ethanol droplet and spray using non-ideal vapour-liquid equilibrium models. 2021 , 168, 120876		3
361	Temperature Effect on the Liquid Liquid Equilibrium of Isopropanol + Trisodium Citrate + Water Aqueous Two-Phase Systems at T = 288.15, 298.15, 308.15, and 318.15 K. <i>Journal of Chemical & Engineering Data</i> , 2021 , 66, 2050-2060	2.8	3
360	Densities, speeds of sound and molar heat capacities of multicomponent liquid mixtures containing 1-methylpiperidine, pyrrolidin-2-one and cycloalkanones at varying temperatures. 2021 , 156, 106389		1
359	Use of Partial Molal Enthalpy for Refining the Partition of Water Activity into Electrostatic and Nonelectrostatic Components. 2021 , 50, 752-770		
358	Analysis of Data on VaporIliquid Equilibrium in Multicomponent Systems Using Artificial Neural Networks. <i>Theoretical Foundations of Chemical Engineering</i> , 2021 , 55, 403-409	0.9	1
357	Hygroscopic growth of aerosol particles consisted of oxalic acid and its internal mixture with ammonium sulfate for the relative humidity ranging from 80% to 99.5%. 2021 , 252, 118318		5
356	Drying paths of phase-separating solution coatings exposed to humidity.		O
355	Modeling and parameters estimation for the solubility calculations of nicotinamide using UNIFAC and COSMO-based models. <i>Fluid Phase Equilibria</i> , 2021 , 535, 112970	2.5	5
354	Predicting entropy and heat capacity of hydrocarbons using machine learning. 2021 , 4, 100054		3
353	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	259-92(58 ¹
352	The Representation of Cross Second Virial Coefficients by Multifluid Mixture Models and Other Equations of State. <i>Industrial & Equations of State. Industrial & Equa</i>	3.9	2
351	Development of an Infinite Dilution Activity Coefficient Prediction Model for Organic Solutes in Ionic Liquids with Modified Partial Equalization Orbital Electronegativity Method Derived Descriptors. 2021 , 6, 15361-15373		1
350	Extractive distillation of the benzene and acetonitrile mixture using an ionic liquid as the entrainer. 2021 , 6, 444-451		4

349	Liquid-Liquid Chromatography: Current Design Approaches and Future Pathways. 2021 , 12, 495-518		1
348	Thermodynamic Modeling and Evaluation of Fuel Evaporation in Petrol Engine Tanks. 2021 , 93, 1257-12	66	
347	Comparison of solvent-based affinity separation processes using Cyrene and Sulfolane for aromatic/aliphatic separations. 2021 , 96, 2630-2646		1
346	Thermodynamic Assessment of Chemical Equilibrium for the Synthesis of Solketal in the Liquid Phase. 2021 , 44, 1356-1363		1
345	Assessing the Uncertainties in Ozone and SOA Predictions due to Different Branching Ratios of the Cresol Pathway in the Toluene-OH Oxidation Mechanism. 2021 , 5, 1958-1970		1
344	Prediction of the Synergistic Glass Transition Temperature of Coamorphous Molecular Glasses Using Activity Coefficient Models. 2021 , 18, 3439-3451		O
343	Thermodynamic representation of ionic liquids phase equilibrium with PDH-ASOG and PDH-UNIFAC models. 2021 , 333, 115926		2
342	VaporIliquid Equilibria Prediction and Validation of Binary Systems Containing SiCl4 by Using the MOSCED Model. 2021 , 50, 1037-1050		
341	LIQUID [IQUID EQUILIBRIUM CALCULATIONS OF SYSTEMS CONTAINING VEGETABLE OIL + FATTY ACIDS + ETHANOL + WATER USING NEW PARAMETERS FOR THE UNIFAC SUBGROUPS OF ETHANOL AND WATER. <i>Fluid Phase Equilibria</i> , 2021 , 113182	2.5	0
340	Solid-liquid equilibria for dibenzofuran or Xanthene + Heavy Hydrocarbons: Experimental measurements and modelling. 2021 , 335, 116536		1
339	Aquatic Toxicity Calculation of Mixtures: A Chemical Activity Approach Incorporating a Bioavailability Reduction Concept. 2021 , 55, 11183-11191		1
338	Maximizing Propylene Separation from Propane by Extractive Distillation with Aqueous N-Methyl-2-pyrrolidone as Separating Agent. 2021 , 44, 1726-1736		O
337	Kinetic study on the reaction of p-tert-butylbenzoic acid with methanol catalyzed by deep eutectic solvent based on choline chloride. 2021 , 53, 1241		1
336	Thermodynamic measurement and modeling of hydrate dissociation for CO2/refrigerant + sucrose/fructose/glucose solutions. <i>AICHE Journal</i> , 2021 , 67, e17379	3.6	2
335	Thermodynamics of mixtures containing a fluorinated benzene and a hydrocarbon. 2021 , 335, 116506		1
334	Enhanced thermodynamic modelling for hydrothermal liquefaction. 2021 , 298, 120796		4
333	Development of the NRTL functional activity coefficient (NRTL-FAC) model using high quality and critically evaluated phase equilibria data. 1. <i>Fluid Phase Equilibria</i> , 2021 , 541, 113088	2.5	0
332	Comparisons of Molecular Structure Generation Methods Based on Fragment Assemblies and Genetic Graphs. 2021 , 61, 4245-4258		2

331	Development of a Modified JobackReid Group Contribution Method to Predict the Sooting Tendency of Oxygenated Fuels. 2021 , 35, 13144-13158	2
330	Shortcut Method for the Prediction of the Cocrystal Solubility Line.	5
329	Influence of still design and modelling of the behaviour of volatile terpenes in an artificial model gin. 2021 , 129, 46-64	1
328	Biobased entrainer screening for extractive distillation of acetone and diisopropyl ether. 2021 , 270, 118749	2
327	Water uptake and optical properties of mixed organic-inorganic particles. 1-16	2
326	Identification and Screening of Potential Organic Solvents for the Liquidliquid Extraction of Aromatics.	О
325	Separation of ethanol azeotropic mixture using deep eutectic solvents in liquid-liquid extraction process. 2021 , 338, 116637	1
324	Controlling the Flashpoint of a Flammable Solvent with a Refrigerant. 1	
323	Leveraging De Donder relations for a thermodynamically rigorous analysis of reaction kinetics in liquid media. 2021 ,	2
322	Predicting Activity Coefficients at Infinite Dilution for Varying Temperatures by Matrix Completion. Industrial & Completion Activity Coefficients at Infinite Dilution for Varying Temperatures by Matrix Completion. 3.9	2
321	Dispersion activity coefficient models. Part 3: A topology preserving group contribution model. Fluid Phase Equilibria, 2021, 544-545, 113097	1
320	Calculating the chemical and phase equilibria of mercury in natural gas. <i>Fluid Phase Equilibria</i> , 2021 , 544-545, 113089	Ο
319	Suitable Experimentation-Modeling Binomial to Design the Extraction of an Alkanol with Water in Aqueous Ternary Solutions of Ester-Akanol. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 13938-13949	
318	Application of nature-inspired algorithms with generalized Pitzer-Debye-H dkel (PDH) refinement for liquid liquid equilibria (LLE) correlation in cyclic di-ether systems. <i>AICHE Journal</i> , e17434	О
317	Topological investigations of molecular interactions in binary and ternary mixtures at varying temperatures and atmospheric pressure: Excess molar volumes and excess isentropic compressibilities. 2021 , 35, 100771	
316	Lupane-type triterpenoids from Acacia dealbata bark extracted by different methods. 2021 , 170, 113734	0
315	Solubility in the system acetic acid [h-amyl alcohol [h-amyl acetate [Water at 293.15 K, 303.15 K, 313.15 K and 323.15 K and atmospheric pressure. 2021 , 161, 106515	3

313	trends in solvent impact on infinite dilution activity coefficients of solutes reviewed and visualized using an algorithm to support selection of solvents for greener fluid separations. 2021 , 272, 118727		2
312	Ionic liquid-assisted refinery processes 🖪 review and industrial perspective. 2021 , 302, 121195		6
311	New Association Schemes for Tri-Ethylene Glycol. Fluid Phase Equilibria, 2021, 113254	2.5	1
310	Role of ecosystem-atmosphere exchanges of semi-volatile organic compounds in organic aerosol formation. 2021 , 263, 118541		2
309	Solvent mixtures in pharmaceutical development: Maximizing the API solubility and avoiding phase separation. <i>Fluid Phase Equilibria</i> , 2021 , 548, 113200	2.5	O
308	Tunable naturally-derived oligomeric ionic liquids: phase behavior and liquid crystal profile. <i>Fluid Phase Equilibria</i> , 2021 , 548, 113168	2.5	1
307	Calculation of interfacial tension of binary systems containing water and an organic component by group contribution methods. 2021 , 244, 116796		
306	Separation of NH3/CO2 from melamine tail gas with ionic liquid: Process evaluation and thermodynamic properties modelling. 2021 , 274, 119007		7
305	Transformer-convolutional neural network for surface charge density profile prediction: Enabling high-throughput solvent screening with COSMO-SAC. 2021 , 246, 117002		3
304	Phase equilibria of mixtures involving fatty acid ethyl esters and fat alcohols between 4 and 27 kPa for bioproduct production. 2021 , 306, 121304		1
303	Flash point measurement and prediction of dodecane + ethanol + FAEE systems. 2021 , 306, 121723		1
302	The case for a common software library and a set of enumerated benchmark problems in computer-aided molecular design. 2022 , 35, 100724		O
301	Computer-aided molecular design of solvents for chemical separation processes. 2022 , 35, 100732		3
300	Effective solvent system selection in the recrystallization purification of pharmaceutical products. <i>AICHE Journal</i> , 2021 , 67, e17169	3.6	3
299	The RCF biorefinery: Building on a chemical platform from lignin. 2021 , 241-297		3
298	The universal recovery strategy. 2021 , 51-68		
297	An empirical model for solvation based on surface site interaction points. 2021 , 12, 13193-13208		1
296	Propelling microdroplets generated and sustained by liquid-liquid phase separation in confined spaces. 2021 , 17, 5362-5374		6

295	Molecular Thermodynamics for Pharmaceutical Process Modeling and Simulation. 505-519	1
294	Optimization-Based Approaches to Computational Molecular Design. 173-193	1
293	Computer-Aided Methodologies for the Design of Reaction Solvents. 267-305	3
292	Phase Equilibria in Fluid Systems. 173-321	1
291	Modeling the Non-ideal Thermodynamics of Mixed Organic/Inorganic Aerosols. 2007, 782-786	1
290	Subsurface Processes of Nonaqueous Phase Contaminants. 1989 , 237-254	2
289	Structural Models of Catalytic Cracking Chemistry: A Case Study of a Group Contribution Approach to Lumped Kinetic Modeling. 1991 , 101-125	6
288	Development of a Numerically Efficient Biodiesel Decanter Simulator. 2015 , 85-105	1
287	Physico-Chemical Interactions in the Flavor-Release Process. 2017 , 35-36	4
286	Microbial Processes. 2007, 575-597	2
286	Microbial Processes. 2007, 575-597 Introduction. 2011, 1-3	1
285	Introduction. 2011, 1-3	1
285	Introduction. 2011, 1-3 Basic Principles of Extraction with Dense Gases. 1988, 8-31	1
285 284 283	Introduction. 2011, 1-3 Basic Principles of Extraction with Dense Gases. 1988, 8-31 Dortmunder Datenbank [Organisation, Stand und Anwendungsm [Glichkeiten. 1987, 153-164]	1 1
285 284 283 282	Introduction. 2011, 1-3 Basic Principles of Extraction with Dense Gases. 1988, 8-31 Dortmunder Datenbank [Drganisation, Stand und Anwendungsm [] glichkeiten. 1987, 153-164 Industrial Use of Group Contribution Methods for Estimation of Physical Properties. 1988, 349-382	1 1 1
285 284 283 282	Introduction. 2011, 1-3 Basic Principles of Extraction with Dense Gases. 1988, 8-31 Dortmunder Datenbank © Drganisation, Stand und Anwendungsm © Glichkeiten. 1987, 153-164 Industrial Use of Group Contribution Methods for Estimation of Physical Properties. 1988, 349-382 Prediction of Mixture Properties Using UNIFAC. 1988, 405-419	1 1 1 1

277	Thermodynamik der Gemische. 1988 , 1-208		1
276	Water Sorption Thermodynamics in Polymer Matrices. 2014 , 15-45		6
275	Thermodynamic Properties for Water Removal Processes in Solid and Liquid Foods. 1989 , 157-175		2
274	Estimating Binding Coefficients of Chlorinated Aromatics and Aquatic Humic Substances from Molecular Properties. 1991 , 437-443		1
273	Designining Environmentally Benign Solvent Substitutes. 1999 , 317-331		2
272	Design of Reaction Medium for Nonaqueous Biocatalysis: Analysis on Enzyme Hydration and Catalytic Activity in Organic Solvent. 1994 , 481-484		1
271	Properties. 2005 , 390-425		4
270	Benzyltoluene/dibenzyltoluene-based mixtures as suitable liquid organic hydrogen carrier systems for low temperature applications. 2020 , 45, 14897-14906		29
269	Partitioning of amylase produced by Aspergillus niger in solid state fermentation using aqueous two-phase systems. 2020 , 94, 116-125		3
268	Generalized Chemical Equilibrium Constant of Formaldehyde Oligomerization. <i>Industrial & Engineering Chemistry Research</i> , 2020 , 59, 11431-11440	3.9	5
267	Isobaric VaporDiquid Equilibria of Binary Mixtures of Valerolactone + Acetone and Ethyl Acetate. <i>Journal of Chemical & Data</i> , 2020, 65, 419-425	2.8	3
266	Chapter 8:SAFT Associating Fluids and Fluid Mixtures. 2010 , 215-279		47
265	SCARABEUS: Supercritical carbon dioxide/alternative fluid blends for efficiency upgrade of solar power plants. 2020 ,		2
264	Statistical Thermodynamic Calculations of the Hydrogen Bonding, Dipolar, and Dispersion Solubility Parameters. 2007 , 45-73		1
263	The Hansen Solubility Parameters (HSP) in Thermodynamic Models for Polymer Solutions. 2007 , 75-94		3
262	Solubility in Water. 2000 ,		1
261	Thermodynamics of Polymer Solutions. 2002 ,		1
2 60	Introduction. 2006 , 1-59		1

259	Biodiesel Process Design through a Computer-aided Molecular Design Approach. 2009 , 979-986	2
258	Recovery of aroma compounds from orange essential oil. 2000 , 17, 705-712	22
257	Prediction of electrolyte vapor-liquid equilibrium by UNIFAC-Dortmund. 2001 , 18, 127-137	16
256	A THERMODYNAMIC MODEL TO PREDICT WAX FORMATION IN PETROLEUM FLUIDS. 2001 , 18, 411-422	15
255	An empirical method to correlate and predict solute distribution in ternary liquid-liquid systems. 2002 , 19, 343-353	1
254	Vapor-liquid equilibrium measurements for the binary system methyl acetate+ethanol at 0.3 and 0.7 MPa. 2011 , 28, 325-332	7
253	Liquid-Liquid Equilibrium Data for the Ternary Systems of Palm Oil + Ethyl Lactate + Phytonutrients (Carotenes and Tocols) at 303.15 K. 2017 , 8, 215-220	3
252	Group contribution methods for estimating the properties of polymer systems. 2006 , 60, 287-305	6
251	Isobaric vapour-liquid equilibrium calculations of binary systems using neural network. 2004 , 69, 669-674	10
250	Empirical Fundamental Equations of State for Pure Fluids and Mixtures. 2020 , 365-407	7
250	Empirical Fundamental Equations of State for Pure Fluids and Mixtures. 2020 , 365-407 Modelling of multi-component droplet evaporation under cryogenic conditions. 2020 , 75, 81	7 3
249	Modelling of multi-component droplet evaporation under cryogenic conditions. 2020 , 75, 81	3
249	Modelling of multi-component droplet evaporation under cryogenic conditions. 2020 , 75, 81 Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. 2021 , 9, 71 Characterization of Feed Properties for Conceptual Process Design Involving Complex Mixtures,	3
249 248 247	Modelling of multi-component droplet evaporation under cryogenic conditions. 2020 , 75, 81 Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. 2021 , 9, 71 Characterization of Feed Properties for Conceptual Process Design Involving Complex Mixtures, Such as Natural Extracts. 2012 , 03, 836-850 Numerical Investigation of the Influence of Oil Dilution on the Ability to Initiate a Pre-Ignition	3 34 14
249 248 247 246	Modelling of multi-component droplet evaporation under cryogenic conditions. 2020, 75, 81 Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. 2021, 9, 71 Characterization of Feed Properties for Conceptual Process Design Involving Complex Mixtures, Such as Natural Extracts. 2012, 03, 836-850 Numerical Investigation of the Influence of Oil Dilution on the Ability to Initiate a Pre-Ignition Combustion.	3 34 14 2
249 248 247 246 245	Modelling of multi-component droplet evaporation under cryogenic conditions. 2020, 75, 81 Molecular Dynamics Simulations in Drug Discovery and Pharmaceutical Development. 2021, 9, 71 Characterization of Feed Properties for Conceptual Process Design Involving Complex Mixtures, Such as Natural Extracts. 2012, 03, 836-850 Numerical Investigation of the Influence of Oil Dilution on the Ability to Initiate a Pre-Ignition Combustion. Flamma: A flash point prediction tool for biofuels. 2020, 20, 253-254 A Study of the Gas Liquid Partition Coefficients of Eleven Normal, Branched and Cyclic Alkanes in	3 34 14 2

241	Relating hygroscopicity and composition of organic aerosol particulate matter.	4
240	A two-dimensional volatility basis set: 1. organic-aerosol mixing thermodynamics.	5
239	New and extended parameterization of the thermodynamic model AIOMFAC: calculation of activity coefficients for organic-inorganic mixtures containing carboxyl, hydroxyl, carbonyl, ether, ester, alkenyl, alkyl, and aromatic functional groups.	3
238	The sensitivity of secondary organic aerosol (SOA) component partitioning to the predictions of component properties IPart 3: Investigation of condensed compounds generated by a near-explicit model of VOC oxidation.	4
237	Aerosol hygroscopic growth parameterization based on a solute specific coefficient.	1
236	The sensitivity of Secondary Organic Aerosol component partitioning to the predictions of component properties: part 2; determination of particle hygroscopicity and its dependence on "apparent" volatility.	3
235	Modeling the gas-particle partitioning of secondary organic aerosol: the importance of liquid-liquid phase separation.	1
234	Henry's law constants of diacids and hydroxypolyacids: recommended values.	2
233	Model for acid-base chemistry in nanoparticle growth (MABNAG).	1
232	Hygroscopicity of organic compounds from biomass burning and their influence on the water uptake of mixed organic mmonium sulfate aerosols.	2
231	Improved AIOMFAC model parameterisation of the temperature dependence of activity coefficients for aqueous organic mixtures.	1
230	Hygroscopic behavior of multicomponent organic aerosols and their internal mixtures with ammonium sulfate.	7
229	Closure between measured and modelled particle hygroscopic growth during TORCH2 implies ammonium nitrate artefact in the HTDMA measurements.	4
228	Effects of uncertainties in the thermodynamic properties of aerosol components in an air quality model Part I: Treatment of inorganic electrolytes and organic compounds in the condensed phase.	1
227	A thermodynamic model of mixed organic-inorganic aerosols to predict activity coefficients.	4
226	Do atmospheric aerosols form glasses?.	9
225	Organic particulate matter formation at varying relative humidity using surrogate secondary and primary organic compounds with activity corrections in the condensed phase obtained using a method based on the Wilson equation.	14
224	Amorphous and crystalline aerosol particles interacting with water vapor IPart 1: Microstructure, phase transitions, hygroscopic growth and kinetic limitations.	4

223	Treatment of non-ideality in the SPACCIM multiphase model Part 1: Model development. 2016, 9, 247-281	6
222	The Secondary Organic Aerosol Processor (SOAP v1.0) model: a unified model with different ranges of complexity based on the molecular surrogate approach.	2
221	Prediction of cloud condensation nuclei activity for organic compounds using functional group contribution methods.	1
220	Determination of the Surface Free Energy of Solids. 2013 , 1, 3-45	56
219	Calculation and Measurement of Flash Point for n-Decane + n-Octanol and Acetic Acid + n-Butanol Using a Tag-Open-Cup Apparatus. 2015 , 29, 45-50	2
218	Glycerol Viable Solvent for Absorption of Highly Polar Solutes I: Behaviour of Molecular Interactions. 2015 , 3, 282-286	3
217	Study of Thermodynamic Modeling of Isothermal and Isobaric Binary Mixtures in Vapor-Liquid Equilibrium (VLE) of Tetrahydrofuran with Benzene (303.15 K) Cyclohexane (333.15 K), Methanol (100 kPa). 2021 , 1, 286-296	
216	Isobaric VaporDiquid Equilibrium Data for the IsopropanolWater System. <i>Journal of Chemical & 2.8</i>	1
215	Simulation of the deasphalting process of crude oils: Models development and extraction conditions analysis. 2021 , 109615	
214	Dissipative particle dynamics simulations in colloid and Interface science: a review. 2021 , 298, 102545	7
213	FORest Canopy Atmosphere Transfer (FORCAsT) 2.0: model updates and evaluation with observations at a mixed forest site. 2021 , 14, 6309-6329	1
212	Modeling the solubility of carbon dioxide in the MDEA + AEEA aqueous solution using the SAFT-HR equation of state and extended UNIQUAC model. 2021 , 1-17	2
211	A Database of Experimentally Derived and Estimated OctanolAir Partition Ratios (KOA). 2021, 50, 043101	7
210	Technische Thermodynamik. 2000, 787-862	
209	Gemische und chemische Reaktionen. 2000 , 237-376	
208	WATER ACTIVITY MEASUREMENTS OF MALONIC ACID AND MALIC ACID. 2001 , 32, 921-922	
207	Gemische und chemische Reaktionen. 2002 , 237-376	
206	Grundlagen der Trennprozesse. 2002 , 275-351	O

205	Deodorization. 2002,
204	Design of Compounds for Physical Methods.
203	Lipase-Catalyzed Condensation in an Organic Solvent. 2005 , 10-1-10-15
202	Bioreactor Analysis and Design. 2006 , 479-514
201	Prediction of Activities of Small Molecules in Polymer Membrane Materials Using the Group Contribution Equation of State. 2006 , 39, 1145-1153
200	Chlorobenzenes and Other Halogenated Mononuclear Aromatics. 2006 , 1258-1477
199	Cloud condensation nucleus (CCN) behavior of organic aerosol particles generated by atomization of water and methanol solutions.
198	Influence of non-ideality on aerosol growth.
197	Homogeneous vs. heterogeneous nucleation in water-dicarboxylic acid systems.
196	Composition and properties of atmospheric particles in the eastern Atlantic and impacts on gas phase uptake rates.
195	Chapter 20:Exposure Modelling for Risk Assessment. 2010 , 508-530
194	The sensitivity of secondary organic aerosol component partitioning to the predictions of component properties Part 1: A systematic evaluation of some available estimation techniques.
193	Modeling secondary organic aerosol formation from isoprene oxidation under dry and humid conditions.
192	Temperature-induced volatility of molecular markers in ambient airborne particulate matter.
191	From Atomistic Calculations to Thermodynamic Quantities. 2011 , 5-41
190	Delhitions and the 1st Law of Thermodynamics. 2011 , 23-80
189	Molecular Modeling of Formulated Consumer Products. 195-206
188	Modeling of Crystallization Processes. 239-285

Parameterising secondary organic aerosol from binene using a detailed oxidation and aerosol 187 formation model. Mass-based hygroscopicity parameter interaction model and measurement of atmospheric aerosol 186 water uptake. Extraction Process Design. 871-918 185 1 Advances and Challenges in Thermal Processing with Flexible Packages. 2013, 197-207 184 Theoretical Tools to Predict Physicochemical Properties of Industrial Foods and Cultivation Media. 183 2013. 89-120 Prediction of Isothermal Vaporliquid Equilibria of Binary Systems by Using Wilson Equation with 182 Parameters Estimated from Pure-Component Properties. 2014, 47, 801-804 181 Steam Stripping Organic Compounds from Contaminated Waters. 1987, 513-519 180 Estimation of Properties from NMR Characterizations. 1987, 1, 163-184 Grundlagen der Extraktion mit verdichteten Gasen. 1987, 10-36 179 178 ANALYSIS OF THE DYNAMIC BEHAVIOR OF DISTILLATION TRAINS. 1988, 105-110 Experience with the Development of a Group-Contribution Equation of State for the Prediction of 177 Physical Properties for Process Engineering Purposes. 1988, 383-403 Uses and Needs of Thermodynamics in the Oil Industry. 1991, 257-276 176 Technische Thermodynamik. 1991, 745-792 175 Thermodynamik der Gemische. 1992, 1-208 174 Low Pressure Vapor-Liquid Equilibrium. 1993, 435-509 173 Choosing a solvent [practical advice. 1996, 48-69] 172 Thermodynamik der Gemische. 1999, 1-244 171 Experimental determination of the temperature dependence of water activities for a selection of 170 aqueous organic solutions.

Modeling of Crystallization Processes. 239-285

168	Bibliography. 2015 , 89-95		
167	Treatment of non-ideality in the multiphase model SPACCIM Part 1: Model development.		0
166	UManSysProp: an online facility for molecular property prediction and atmospheric aerosol calculations.		O
165	- Molecular Thermodynamic Modeling of Fluctuation Solution Theory Properties. 2016 , 252-283		
164	EXTRA□□Ď L□ĎUIDO-L□ĎUIDO APLICADA AO PROCESSO DE REFINO DE ETANOL COMBUST□ŬEL.		
163	Solubility Thermodynamics of Organic Energetic Materials. 2017, 43-62		1
162	PREDIO DA CURVA DE DISSOCIA DE HIDRATOS USANDO METANOL COMO INIBIDOR PELA EQUADO PR-LCVM-UNIFAC.		
161	Stoffmodelle der Technischen Thermodynamik. 2019 , 1-29		
160	D5.1 Dampf-Fl□ Bsigkeits-Gleichgewichte von Mehrkomponenten-Gemischen. 2019 , 603-620		
159	Determining Activity Coefficients of SOA from Isothermal Evaporation in a Laboratory Chamber. 2021 , 8, 212-217		0
158	Critical Assessment of the Thermodynamics in Acidic Resin-Catalyzed Esterifications. <i>Industrial</i> & amp; Engineering Chemistry Research, 2020 , 59, 22079-22091	3.9	1
157	Sorption thermodynamics of low molecular weight compounds in polymers. 2021 , 9, 69-177		
156	Computer-aided design and solvent selection for organic paint and coating formulations. 2022 , 162, 106568		O
155	Thermodynamische Eigenschaften homogener Mischungen. 2020 , 255-346		
154	Fundamentals of Multiphase Chemical Reactions. 2020 , 13-105		
153	The CHIMERE v2020r1 online chemistry-transport model. 2021 , 14, 6781-6811		4
152	Gemische und chemische Reaktionen. 2005 , 237-377		

151 Gemische und chemische Reaktionen. **2006**, 235-375

150	Cubic Equations of State. 2021 , 41-107		
149	Technical note: Estimating aqueous solubilities and activity coefficients of mono- and <i></i> , <i>\lambdalt;i>\lambdalt;i>\lambdalt;i\lambdalt;\lambdalt</i>		3
148	Optimization of quality, safety and health aspects in personal care product preservative design. 2022 , 157, 246-253		1
147	Kinetics Assessment of the Homogeneously Catalyzed Hydroformylation of Ethylene on an Rh Catalyst. <i>Industrial & Engineering Chemistry Research</i> , 2021 , 60, 16665-16681	3.9	O
146	Activity Coefficients from an Equation of State: Novel Approach for Fast Phase Equilibrium Calculations. <i>Industrial & Engineering Chemistry Research</i> ,	3.9	2
145	Highly efficient absorption of methyl tert-butyl ether with ionic liquids. 2021, 282, 120108		1
144	Computer-Aided Framework for the Design of Optimal Bio-Oil/Solvent Blend with Economic Considerations. 2021 , 9, 2159		O
143	Novel Design, Validation, and Optimization of Hydrogen Production with CO 2 Capture Through an Integration of Glycerol Steam Reforming and Pressure Swing Adsorption. SSRN Electronic Journal,	1	
142	Simulation and Modelling of Polymers. 2021 , 205-265		
141	Predictive molecular thermodynamic models for ionic liquids. AICHE Journal,	3.6	2
140	Optimal computer-aided molecular design of ionic liquid mixtures for post-combustion carbon dioxide capture. 2022 , 157, 107622		1
139	Preparation of defect-free asymmetric gas separation membranes with dihydrolevoglucosenone (CyreneTM) as a greener polar aprotic solvent. 2022 , 644, 120173		О
138	Mutual diffusion coefficients of dimethyl carbonate + n-heptane and dimethyl carbonate + isooctane from 288.15 K to 318.15 K. 2022 , 167, 106716		Ο
137	Isobaric vapor-liquid equilibrium for ethanol/water and binary linear siloxane mixtures at 100 kPa. <i>Fluid Phase Equilibria</i> , 2022 , 556, 113371	2.5	О
136	Group contribution-based LCA models to enable screening for environmentally benign novel chemicals in CAMD applications. <i>AICHE Journal</i> , 2022 , 68,	3.6	1
135	Assessment of liquid-liquid equilibrium data by solving the Gibbs-Duhem equation. AICHE Journal,	3.6	0
134	Extension of the AIOMFAC model by iodine and carbonate species: applications for aerosol acidity and cloud droplet activation. 2022 , 22, 973-1013		1

133 The effects of polar solvents on structural, electronic, and optical properties of organic dyes.

132	Experimental study of pressure drop during water than ol condensation in a vertical plate heat exchanger. 1		О
131	Synthesis of methyl cinnamate catalyzed by deep eutectic solvents based on choline chloride: kinetic studies. 1		1
130	Methods for Interpreting the Partitioning and Fate of Petroleum Hydrocarbons in a Sea Ice Environment 2022 ,		O
129	Modelling solubility in semi-crystalline polymers: a critical comparative review. <i>Fluid Phase Equilibria</i> , 2022 , 113412	2.5	2
128	Rational Design and Screening of Ionic Liquid Absorbents for Simultaneous and Stepwise Separations of SO2 and CO2 from Flue Gas. <i>Industrial & Engineering Chemistry Research</i> ,	3.9	O
127	Graph Neural Networks for the prediction of infinite dilution activity coefficients.		1
126	Estimating Inhalation Exposure Resulting from Evaporation of Volatile Multicomponent Mixtures Using Different Modelling Approaches 2022 , 19,		2
125	Interactions of Crosslinked Polyacrylic Acid Polyelectrolyte Gels with Nonionic and Ionic Surfactants 2021 , 125, 13817-13828		1
124	Making thermodynamic models of mixtures predictive by machine learning: matrix completion of pair interactions.		O
123	Reactive Distillation Applied to Biodiesel Production by Esterification: Simulation Studies.		
122	Predictive Approach for the Solubility and Permeability of Binary Gas Mixtures in Glassy Polymers Based on an NETGP-NRHB Model. <i>Industrial & Engineering Chemistry Research</i> , 2022 , 61, 3439-3456	3.9	2
121	A review of the contributions of P. Raj Bishnoi to chemical engineering.		0
120	Prediction of the ASTM and TBP distillation curves and specific gravity distribution curve for fuels and petroleum fluids.		1
119	A predictive viscosity model for aqueous electrolytes and mixed organic[horganic aerosol phases. 2022 , 22, 3203-3233		3
118	Isobaric Vapor[liquid Equilibria for Binary Mixtures of Adiponitrile + 2-Methylglutaronitrile and Adiponitrile + Trans-3-pentenenitrile at 5 kPa and 10 kPa. <i>Journal of Chemical & Dournal of Chemical & Dournal Data</i> ,	2.8	
117	Infinite Dilution Activity Coefficient Measurements for 1-Methyl-4-(1-methylethenyl)-cyclohexene as a Green Solvent for Separation. <i>Journal of Chemical & Description of Chemical & Description Data</i> ,	2.8	1
116	Liaw-UNIFAC flash point model for alcohols-kerosene/diesel fuel blends using average fuel structure. 2022 , 160, 400-410		О

115	SAFT - Mie model for ionic liquids. AICHE Journal,	3.6
114	Thermodynamic modeling of pharmaceuticals solubility in pure, mixed and supercritical solvents. 2022 , 353, 118809	2
113	Message-passing neural network based multi-task deep-learning framework for COSMO-SAC based Eprofile and VCOSMO prediction. 2022 , 254, 117624	3
112	Cholesterol thermodynamic behaviour in mixtures with medium chain fatty acids and vegetable oils composed of them. <i>Fluid Phase Equilibria</i> , 2022 , 557, 113432	2.5 0
111	Model-based compositional predictions for a differential scanning calorimetry/thermogravimetric analysis-mass spectrometry system used for heat of vaporization measurements. 2022 , 318, 123550	
110	Phase behavior of the oleic acid Imethanol Imethyl oleate Iwater mixture as a promising model system for biodiesel production: Brief data review and new results at 303.15 K and atmospheric pressure. 2022 , 319, 123730	2
109	Prediction of small-molecule compound solubility in organic solvents by machine learning algorithms 2021 , 13, 98	O
108	Separation of the Azeotropic Mixture Methanol and Toluene Using Extractive Distillation: Entrainer Determination, Vapor-Liquid Equilibrium Measurement, and Modeling 2021 , 6, 34736-34743	1
107	FloryHuggins Parameters for Thiol-ene Networks Using Hansen Solubility Parameters. 2021 , 54, 11439-	-11448 1
106	Systematic analysis of additives on the performance parameters of sCO2 cycles and their individual effects on the cycle characteristics. 2022 , 123957	O
105	Modelling aerosol molecular markers in a 3D air quality model: Focus on anthropogenic organic markers 2022 , 155360	О
104	Work relation for determining the mixing free energy of small-scale mixtures. 2022, 4,	O
103	Experimental Measurement and Thermodynamic Modeling of the Wax Disappearance Temperature (WDT) for a Quaternary System of Normal Paraffins.	
102	Current Trends in Predictive Methods and Electrolyte Equations of State.	1
101	Chemistry Across Multiple Phases (CAMP) version 1.0: an integrated multiphase chemistry model. 2022 , 15, 3663-3689	1
100	Isobaric vapour-liquid equilibrium of Eerpineol highly diluted in hydroalcoholic mixtures at 101.3 kPa: Experimental measurements and thermodynamic modeling. 2022 , 171, 106806	1
99	A temperature-independent prediction model predicts the vapor-liquid equilibrium of CO2-based binary mixtures. 2022 ,	0
98	Ionic Liquids Design Methodology for Separation Processes. 2021 , 1-8	

97	Prediction of Henry's Law Constants by Matrix Completion. AICHE Journal,	3.6	2
96	Thermodynamically predicting liquid/solid phase change of long-chain fatty acid methyl esters (FAMEs) and its application in evaluating the low-temperature performance of biodiesel. 2022 , 135, 10	4384	O
95	Application of Artificial Neural Networks for the Analysis of Data on Liquid Liquid Equilibrium in Three-Component Systems. <i>Theoretical Foundations of Chemical Engineering</i> , 2022 , 56, 200-207	0.9	
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	O
93	Vapor��iquid Equilibrium Study of the Monochlorobenzene��,6-Dichloropyrimidine Binary System. 2022 , 7, 17670-17678		
92	Phase behaviour and pH-solubility profile prediction of aqueous buffered solutions of ibuprofen and ketoprofen. <i>Fluid Phase Equilibria</i> , 2022 , 560, 113504	2.5	O
91	Bio-additives from glycerol acetylation with acetic acid: Chemical equilibrium model. <i>Results in Engineering</i> , 2022 , 100502	3.3	О
90	Insights on the potential of natural deep eutectic solvents (NADES) to fine-tune durian seed gum for use as edible food coating. <i>Food Hydrocolloids</i> , 2022 , 132, 107861	10.6	2
89	Vapour-Liquid Equilibrium for Xylenes + Tetrapropylene Glycol Binary Systems: Experimental Data and Regression. SSRN Electronic Journal,	1	
88	Application of a First Principles Mathematical Model of a Mass-Transfer Technological Process to Improve the Accuracy of the Estimation of the End Product Quality. <i>Theoretical Foundations of Chemical Engineering</i> , 2022 , 56, 371-387	0.9	
87	Effect of Temperature on the Phase Equilibria of Poly(vinylpyrrolidone) 10000 + Trilithium Citrate + Water Aqueous Two-Phase System and Partitioning of Curcumin at T = 298.15, 308.15, and 318.15 K. <i>Journal of Chemical & Data</i> ,	2.8	1
86	Comparison of UNIFAC and LSER Models for Calculating Partition Coefficients in the HexaneAcetonitrile System Using Middle Distillate Petroleum Products as an Example. <i>Industrial & Mamp; Engineering Chemistry Research</i> , 2022 , 61, 9575-9585	3.9	4
85	Solid-liquid equilibrium of free form of oil contaminants (3-MCPD and glycidol) in lipidic systems. <i>Food Research International</i> , 2022 , 111740	7	
84	Dynamic Modeling of Modified Styrene-Acrylonitrile Process. 2022 , 55, 272-277		
83	Aerosol processes. 2022 , 135-185		
82	Applications of an Association Activity Coefficient Model, NRTL-PA, to Alcohol-Containing Mixtures.		3
81	Simultaneous Solvent Selection and Process Design for Continuous Reaction Extraction Trystallization Systems. 2022 , 61, 11504-11517		O
80	Thermodynamics, Nonideal Mixing, and Phase Separation. 2022 , 78-132		

79	Evaluation of Predictive Solubility Models in Pharmaceutical Process Development-an Enabling Technologies Consortium Collaboration.	
78	Estimation of activity coefficients for aqueous organic redox-flow batteries: Theoretical basis and equations. 2022 , 104901	Ο
77	Hybrid modeling approach for polymer melt index prediction.	
76	Viscosity of Binary Aqueous Solutions Involving Malonic, Maleic, Malic, Tartaric, and Citric Acids in the Temperature Range between 303 and 363 K: Experimental Data and Modeling.	
75	CO2 solubility modelling in Non-Precipitating aqueous solutions of potassium lysinate. 2022 , 300, 121855	0
74	Beyond activity coefficients with pairwise interacting surface (COSMO-type) models. 2022 , 113611	О
73	Efficient Implementation of Wertheim Theory: 2. Master Equations for Asymmetric Solvation.	1
72	Thermodynamic behaviour of an e-cigarette: Investigation of nicotine delivery consistency using nicotine yield. 2022 , 35, 101452	O
71	Prediction of the solubility of organic compounds in high-temperature water using machine learning. 2022 , 190, 105733	1
70	Activity coefficients at infinite dilution via a perturbation method of NRHB model. 2022 , 262, 118043	2
69	A new molecular thermodynamic model of liquid-liquid interfacial tension. 2023 , 564, 113593	О
68	A SMILE is all you need: Predicting limiting activity coefficients from SMILES with natural language processing.	1
67	Optimizing the selection of drug-polymer-water formulations for spray-dried solid dispersions in pharmaceutical manufacturing. 2022 , 2185-2190	О
66	Prediction of Azeotrope Formation in Binary Mixtures with Pure Component Properties and Limiting Activity Coefficients.	Ο
65	Model-based solvent selection for integrated synthesis, crystallisation and isolation processes. 2022 , 601-606	О
64	Stoffmodelle der Technischen Thermodynamik. 2022 , 485-513	Ο
63	Solvent selection for chemical reactions toward optimal thermodynamic and kinetic performances: Group contribution and COSMO-based modeling. 2023 , 564, 113623	Ο
62	Modelling Sorption and Transport of Gases in Polymeric Membranes across Different Scales: A Review. 2022 , 12, 857	2

61	Parametrization of the NRTL Model with a Multiobjective Approach: Implications in the Process Simulation. 2022 , 2, 267-288	0
60	Synthesis of Methyl Sorbate Catalyzed by Deep Eutectic Solvent Based on Choline Chloride: Kinetics and Optimization.	Ο
59	Thermodynamic Solubility Modeling of 2, 2?, 4, 4?, 6, 6? - Hexanitrostilbene (HNS). 2022, 113627	0
58	Vapor-liquid Equilibrium Experiment and Prediction of Excess Property of New Working Pair CO-[BMP][TfN] in Absorption Refrigeration System. 2022 ,	O
57	Model-based solvent selection for the synthesis and crystallisation of pharmaceutical compounds. 2022 , 264, 118125	0
56	Elements and Chemical Bonds Contribution Estimation of Activity Coefficients in Nonideal Liquid Mixtures. 2022 , 10, 2141	1
55	An Intensified Green Process for the Coproduction of DMC and DMO by the Oxidative Carbonylation of Methanol. 2022 , 10, 2094	2
54	Prediction of Azeotrope Formation in Binary Mixtures with Pure Component Properties and Limiting Activity Coefficients. 2022 , 113664	O
53	Prediction of carbon-dioxide activity coefficient for solubility in ionic liquids using multi non-linear regression analysis 2022 , 137102	O
52	Prediction of solid solubility in supercritical carbon dioxide using a pairwise surface contact equation of state ICOSMO-SAC-Phi. 2022 , 191, 105765	O
51	Artificial neural network modeling on the polymer-electrolyte aqueous two-phase systems involving biomolecules. 2023 , 306, 122624	1
50	Estimation of kinematic viscosities and thermal conductivities for liquid mixtures using ASOG-VLE, ASOG-VISCO and ASOG-ThermConduct models. 2023 , 565, 113668	O
49	Group-Contribution SAFT Equations of State: A Review. 2022 , 113674	1
48	NIST-UNIFAC parametrization for phase equilibrium calculation of mixtures containing lactones. 2022 , 113673	O
47	Modelling changes in glass transition temperature in polymer matrices exposed to low molecular weight penetrants. 2023 , 381,	O
46	Molecule superstructures for computer-aided molecular and process design.	O
45	Prediction of parameters of group contribution models of mixtures by matrix completion.	0
44	Thermodynamics of hydrogen storage: Equilibrium study of the LOHC system indole/octahydroindole. 2023 , 335, 127025	1

43	Vapour-liquid equilibrium for xylenes ´+ ´tetrapropylene glycol binary systems: Experimental data and regression. 2023 , 178, 106973	О
42	Capturing molecular interactions in graph neural networks: a case study in multi-component phase equilibrium.	О
41	Study of modeling of cyclohexanol and polystyrene polymer solution at $T=453.15\%$ and $T=493.15\%$ using UNIFAC-FV. 2022 ,	О
40	Micellar solubilization of binary organic liquid mixtures for surfactant enhanced aquifer remediation.	O
39	Estimating evaporation rates and contaminant air concentrations due to small spills of non-ideal aqueous organic solvent mixtures in a controlled environment. 1-14	О
38	Influence of Recycle Operation on the Catalytic Hydrogenation of CO2 to Long-Chain Hydrocarbons.	O
37	GENerator of reduced Organic Aerosol mechanism (GENOA v1.0): an automatic generation tool of semi-explicit mechanisms. 2022 , 15, 8957-8982	О
36	New interaction parameters from VLE data for group contribution (GC-NRTL) model.	О
35	Simulationsstrategie zur belastbaren Auslegung der Essigs 🛮 🗓 re-R 🖺 🗗 kgewinnung aus Abw 🗈 🗟 sern der industriellen Celluloseacetatherstellung.	О
34	Continuum Modelling and Simulation of Flow Batteries. 2023 , 379-412	О
33	Evaluation of Chemical Functional Group Composition of Jet Fuels Using Two-Dimensional Gas Chromatography.	О
32	Thermodynamics of Hydrogen Storage: Equilibrium Study of Liquid Organic Hydrogen Carrier System 1-Methylindole/octahydro-1-methylindole. 2023 , 3, 45-63	O
31	A Workflow for Crystallization Process Design with Simultaneous Process Optimization and Solvent Selection based on the Perturbed-Chain Statistical Associating Fluid Theory.	О
30	Cubic Plus GE (CPGE): Cubic equation of state with simple mixing rule plus excess Gibbs energy that satisfies low-density condition. 2023 , 113730	O
29	Ionic Liquids Design Methodology for Separation Processes. 2022 , 663-671	О
28	A unified ML framework for solubility prediction across organic solvents.	O
27	Density and Viscosity of Linear Siloxanes and Their Mixtures. 2023 , 68, 314-329	0
26	An Overview of Computer-aided Molecular and Process Design.	0

25	SPT-NRTL: A physics-guided machine learning model to predict thermodynamically consistent activity coefficients. 2023 , 568, 113731	О
24	Characterizing combustion and atomization of PODEn and ethanol/PODEn binary droplets. 2023 , 341, 127672	O
23	Aqueous Two-phase System Separation of Heat-Stable Salt Ions in Flue Gas Desulfurizer. 2023, 30, 29-38	О
22	Solubility of palbociclib in supercritical carbon dioxide from experimental measurement and PengRobinson equation of state. 2023 , 13,	Ο
21	LiquidŪiquid Phase Separation of Two Non-Dissolving Liquids∆ Mini Review. 2023 , 11, 1145	О
20	Flash point of binary and ternary monoterpene mixtures: Experimental and modeling. 2023 , 172, 1048-1057	Ο
19	Enhancing R410A blend separation by using ionic liquids: From UNIFAC model extension, solvent design to molecular dynamics simulation. 2023 , 274, 118709	0
18	Simulation of mercury distribution in an offshore natural gas processing platform. 2023 , 345, 128164	Ο
17	The general formulation of the energy equation and the impact of enthalpy diffusion on multi-component droplet heat and mass transfer. 2023 , 210, 124172	0
16	Graph neural networks for temperature-dependent activity coefficient prediction of solutes in ionic liquids. 2023 , 171, 108153	Ο
15	Modeling and simulation of pervaporation (PV) separation for alcohol dehydration. 2023, 9, e13713	1
14	Prediction of Swelling of Polypropylene Separators and Its Effect on the Lithium-Ion Battery Performance. 2023 , 5, 2026-2031	Ο
13	Direct measurement of the viscosity of ternary aerosol mixtures. 2023 , 3, 595-607	0
12	Effect of temperature and composition on solubility and thermodynamics of salicylic acid in aqueous mixtures of betaine-based deep eutectic solvents. 2023 , 40, 910-924	O
11	Sorption of CO2, CH4 and Their Mixtures in Amorphous Poly(2,6-dimethyl-1,4-phenylene)oxide (PPO). 2023 , 15, 1144	0
10	Rational method for defining and quantifying pseudo-components based on NMR spectroscopy. 2023 , 25, 10288-10300	O
9	New Model to Predict Infinite Dilution Activity Coefficients Based on (p/図)T,x -f0. 2023 , 8, 12439-12444	0
8	Surface tension models for binary aqueous solutions: a review and intercomparison.	Ο

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7	Extraction of valuable chemicals from food waste via computational solvent screening and experiments. 2023 , 316, 123719	O
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5	ŒUNIFAC (□□□□□ ■□□ Online first,	О
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1	Performance of different UNIFAC parameter sets in describing experimental liquid liquid equilibrium data of biodiesel systems. 2023 , 383, 122022	О