Table S1

Pure component parameters of the model for the *n*-alkane series

Component	M_w	m	σ (Å)	ε / k (K)	%AAD[a]		T range (K)	References	
					p^{vap}	v^{liq}		p	v
Methane	16.043	1.0000	3.7037	150.00	0.36	0.98	91-500	43, 44, 50	43-45, 50
Ethane	30.070	1.6903	3.4530	183.21	0.81	1.28	90-500	43, 44, 50	43, 44,46, 49, 50
Propane	44.096	2.1539	3.5259	195.05	1.85	0.65	85-600	43, 44, 50	43, 44, 49, 50
Butane	58.123	2.5858	3.5686	204.28	1.45	0.95	134-573	43, 44, 50	43, 44, 49, 50
Pentane	72.150	3.1134	3.5808	205.77	1.00	1.70	143-573	43,44	43, 44, 47
Hexane	86.177	3.7208	3.5291	204.76	1.55	0.71	173-548	43,44	43, 44, 48
Heptane	100.204	4.1594	3.5675	207.80	1.77	1.06	183-540	43,44	43, 44
Octane	114.231	4.6073	3.5826	210.27	1.72	0.39	216-569	43,44	43, 44
Nonane	128.258	5.1543	3.5661	209.72	1.26	0.35	219-594	43,44	43, 44
Decane	142.850	5.6582	3.5690	210.27	1.59	0.24	243-617	43, 44, 51	43, 44
Undecane	156.312	6.2309	3.5522	209.47	1.65	0.57	247-639	43,44	44
Dodecane	170.338	6.7006	3.5586	210.33	1.67	0.69	263-658	43, 44, 51	43, 44
Tridecane	184.365	7.1945	3.5691	210.56	1.33	0.34	267-675	43,44	43, 44
Tetradecane	198.392	7.5751	3.5814	212.54	1.71	0.91	279-693	43, 44, 51	43, 44
Pentadecane	212.419	7.9508	3.6023	213.99	1.48	0.91	283-708	43,44	43, 44
Hexadecane	226.446	8.4812	3.5896	213.71	2.06	1.41	291-723	43, 44, 51	43, 44
Heptadecane	240.473	8.9459	3.5898	214.14	1.65	1.67	295-736	43,44	43, 44
Octadecane	254.500	9.4384	3.5870	213.99	2.02	1.83	301-747	43, 44, 51	43, 44
Nonadecane	268.527	9.8753	3.6109	214.68	4.51	1.01	305-758	43,44	43, 44
Eicosane	282.553	10.5441	3.5622	213.03	2.33	2.51	309-768	43,44	43, 44

[a] $\%AAD = (100/n)\sum_j^n \left|Cald - Expl\right|_j / Expl_j$

Table S2

The constants of eq 23 in correlating the model parameters as a function of molecular weight (reference $M_{w,\,CH4}$ = 16.043)

Parameter	$q_{0,k}$	$q_{1,k}$	$q_{2,k}$
m/M_w	0.0618	-0.0185	-0.0093
$\sigma(\mathring{A})$	3.6912	-0.3601	0.2895
ε/k (K)	149.7756	74.04143	-6.9680

Table S3

Pure component parameters of the PC-SAFT equation of state for the *n*-alkane series

Component	M_w	m	σ (Å)	ε / k (K)	%AAD[a]		T range (K)	References	
					p^{vap}	v^{liq}		p	v
Methane	16.043	1.0000	3.7037	150.00	0.36	0.98	91-500	43, 44, 50	43-45, 50
Ethane	30.070	1.5769	3.5403	193.99	1.34	1.23	90-500	43, 44, 50	43, 44, 49, 50
Propane	44.096	1.9465	3.6583	211.71	1.77	0.61	85-600	43, 44, 50	43, 44, 49, 50
Butane	58.123	2.2888	3.7317	225.65	1.83	0.87	134-573	43, 44, 50	43, 44,46, 49, 50
Pentane	72.150	2.6870	3.7789	231.76	2.21	1.66	143-573	43,44	43, 44, 47
Hexane	86.177	3.2086	3.7224	231.10	2.67	0.94	173-548	43,44	43, 44, 48
Heptane	100.204	3.5427	3.8040	236.29	2.69	2.66	183-540	43,44	43, 44
Octane	114.231	3.8567	3.8313	241.61	1.52	1.10	216-569	43,44	43, 44
Nonane	128.258	4.3122	3.8153	241.61	2.12	0.62	219-594	43,44	43, 44
Decane	142.850	4.7303	3.8231	242.53	2.68	0.82	243-617	43, 44, 51	43, 44
Undecane	156.312	5.2060	3.8154	241.83	3.40	1.28	247-639	43,44	44
Dodecane	170.338	5.5937	3.8253	243.11	3.60	1.20	263-658	43, 44, 51	43, 44
Tridecane	184.365	5.8190	3.8840	247.19	1.84	1.48	267-675	43,44	43, 44
Tetradecane	198.392	6.0979	3.9102	250.14	2.38	1.26	279-693	43, 44, 51	43, 44
Pentadecane	212.419	6.3725	3.9418	252.44	1.89	1.35	283-708	43,44	43, 44
Hexadecane	226.446	6.8230	3.9235	251.83	2.85	0.89	291-723	43, 44, 51	43, 44
Heptadecane	240.473	7.1315	3.9407	253.42	2.22	0.86	295-736	43,44	43, 44
Octadecane	254.500	7.5826	3.9270	252.44	2.97	0.78	301-747	43, 44, 51	43, 44
Nonadecane	268.527	7.9294	3.9316	253.22	3.28	0.45	305-758	43,44	43, 44
Eicosane	282.553	8.3404	3.9062	253.31	2.86	1.43	309-768	43,44	43, 44

[a] $\%AAD = (100/n)\sum_j^n \left|Cald - Expl\right|_j / Expl_j$

Table S4

The constants of eq 23 in correlating the model parameters as a function of molecular weight (reference $M_{w,\,CH4}$ = 16.043)

Parameter	$q_{0,k}$	$q_{1,k}$	$q_{2,k}$
m/M_w	0.0607	-0.0204	-0.0143
$\sigma(\mathring{A})$	3.7013	-0.2555	0.5513
ε/k (K)	150.1376	93.2707	16.7851

Table S5

Pure component parameters of the PC-SAFT-D equation of state for the *n*-alkane series

Component	M_w	m	σ (Å)	ε / k (K)	%AAD[a]		T range (K)	References	
					p^{vap}	v^{liq}		p	v
Propane	44.096	2.0000	3.6656	208.58	1.77	3.67	85-600	43, 44, 50	43, 44, 49, 50
Butane	58.123	2.3081	3.7102	226.52	1.85	1.17	134-573	43, 44, 50	43, 44,46, 49, 50
Pentane	72.150	2.6747	3.7678	234.23	1.67	1.38	143-573	43,44	43, 44, 47
Hexane	86.177	3.0797	3.7790	237.67	2.97	2.34	173-548	43,44	43, 44, 48
Heptane	100.204	3.3398	3.9007	244.67	3.12	1.08	183-540	43,44	43, 44
Octane	114.231	3.5770	3.9670	251.53	1.71	0.49	216-569	43,44	43, 44
Nonane	128.258	3.8965	3.9981	254.10	2.18	0.65	219-594	43,44	43, 44
Decane	142.850	4.1917	4.0453	256.71	2.28	0.54	243-617	43, 44, 51	43, 44
Undecane	156.312	4.5193	4.0935	257.53	2.82	1.22	247-639	43,44	44
Dodecane	170.338	4.7651	4.1212	260.84	2.76	0.47	263-658	43, 44, 51	43, 44
Tridecane	184.365	4.9485	4.2004	264.67	1.06	1.07	267-675	43,44	43, 44
Tetradecane	198.392	5.1350	4.2480	268.54	1.52	0.77	279-693	43, 44, 51	43, 44
Pentadecane	212.419	5.3355	4.2963	271.21	1.95	0.81	283-708	43,44	43, 44
Hexadecane	226.446	5.6067	4.3143	272.16	1.49	0.60	291-723	43, 44, 51	43, 44
Heptadecane	240.473	5.8116	4.3476	274.48	2.33	0.66	295-736	43,44	43, 44
Octadecane	254.500	6.0659	4.3682	274.96	2.15	0.73	301-747	43, 44, 51	43, 44
Nonadecane	268.527	6.3208	4.4027	275.75	2.59	0.54	305-758	43,44	43, 44
Eicosane	282.553	6.5581	4.4054	276.70	2.55	1.42	309-768	43,44	43, 44

[a] $\%AAD = (100/n)\sum_j^n \left| Cald - Expl \right|_j / Expl_j$

Table S6

The constants of eq 23 in correlating the model parameters as a function of molecular weight (reference $M_{w,\ C3H8} = 44.096$)

Parameter	$q_{0,k}$	$q_{1,k}$	$q_{2,k}$
m/M_w	0.0444	-0.0188	-0.0090
$\sigma(\mathring{A})$	3.6974	0.2493	0.8200
ε/k (K)	211.0671	58.6695	26.1455