

# SUPPLEMENTARY TABLES

**Table S1: Predicted Heat of Vaporization of Training and Validation Data Set of Pure Hydrocarbons using Developed Two and Three Parameter Models (Eqns. 8 and 9) versus the Experimental Heat of Vaporization Values**

Index of data	Hydrocarbon	T <sub>b</sub> (K)	S(-)	M (g/g-mol)	Expt. ΔH <sup>vap</sup> (kJ/g-mol)	Pred.ΔH <sup>vap</sup> (kJ/g-mol) Eqn. 8	% Error	Pred.ΔH <sup>vap</sup> (kJ/g-mol) Eqn. 9	% Error
<b>Training data set of Pure Hydrocarbons</b>									
1	Propane <sup>#</sup>	231.1	0.508	44.1	19.04	17.81	-6.48	17.64	-7.33
3	iso-Butane <sup>#</sup>	261.3	0.564	58.1	21.30	20.47	-3.89	20.50	-3.76
4	n-Pentane <sup>#</sup>	309.2	0.631	72.2	25.79	25.44	-1.36	25.29	-1.93
6	2,2-dimethyl propane <sup>#</sup>	282.7	0.597	72.2	22.74	22.34	-1.78	22.60	-0.61
7	n-Hexane <sup>#</sup>	341.9	0.664	86.2	28.85	28.92	0.25	28.74	-0.37
8	iso-Hexane <sup>#</sup>	333.4	0.658	86.2	27.79	27.84	0.18	27.82	0.12
9	3-methyl pentane <sup>#</sup>	336.4	0.669	86.2	28.06	28.13	0.23	28.09	0.11
10	2,2-Dimethyl butane <sup>#</sup>	322.9	0.655	86.2	26.31	26.47	0.63	26.67	1.35
12	n-Heptane <sup>#</sup>	371.6	0.689	100.2	31.77	32.19	1.34	31.98	0.67
13	2-Methyl hexane <sup>#</sup>	363.2	0.684	100.2	30.62	31.09	1.54	31.05	1.39
14	3-Methyl hexane <sup>#</sup>	365.0	0.692	100.2	30.89	31.25	1.16	31.20	1.00
15	3-Ethyl pentane <sup>#</sup>	366.6	0.703	100.2	31.12	31.34	0.72	31.31	0.61
16	2,2-Dimethyl pentane <sup>#</sup>	352.4	0.679	100.2	29.23	29.67	1.52	29.84	2.09
18	2,4-Dimethyl pentane <sup>#</sup>	352.4	0.678	100.2	29.55	29.68	0.45	29.85	1.01
19	3,3-Dimethyl pentane <sup>#</sup>	352.4	0.698	100.2	29.62	29.47	-0.50	29.72	0.33
20	2,2,3-Trimethyl <sup>#</sup>	352.4	0.695	100.2	28.90	29.50	2.08	29.74	2.89
21	n-Octane <sup>#</sup>	398.8	0.707	114.2	34.41	35.29	2.57	35.04	1.84
22	2-Methyl heptane <sup>#</sup>	390.8	0.703	114.2	33.26	34.21	2.86	34.13	2.61
24	4-Methyl heptane <sup>#</sup>	390.9	0.709	114.2	33.35	34.15	2.41	34.10	2.24
26	2,2-Dimethyl hexane <sup>#</sup>	382.0	0.700	114.2	32.07	33.02	2.96	33.12	3.27
28	2,4-Dimethyl hexane <sup>#</sup>	382.6	0.705	114.2	32.51	33.04	1.64	33.15	1.98
29	2,5-Dimethyl hexane <sup>#</sup>	382.3	0.698	114.2	32.54	33.08	1.67	33.17	1.93
30	3,3-Dimethyl hexane <sup>#</sup>	385.1	0.715	114.2	32.31	33.28	2.99	33.37	3.29
32	3-Ethyl-2-methyl pentane <sup>#</sup>	388.8	0.724	114.2	32.93	33.68	2.29	33.74	2.47
33	3-Ethyl-3-methyl pentane <sup>#</sup>	391.4	0.732	114.2	32.78	33.95	3.58	33.99	3.70
34	2,2,3-Trimethyl pentane <sup>#</sup>	383.0	0.721	114.2	31.94	32.92	3.06	33.09	3.59
36	2,3,3-Trimethyl pentane <sup>#</sup>	387.9	0.731	114.2	32.12	33.48	4.23	33.59	4.58
37	2,3,4-Trimethyl pentane <sup>#</sup>	386.6	0.724	114.2	32.36	33.38	3.15	33.49	3.48
38	n-Nonane <sup>#</sup>	426.5	0.722	128.3	36.39	38.59	6.04	38.25	5.10
40	n-Dodecane <sup>#</sup>	487.5	0.753	170.3	43.31	45.81	5.76	45.51	5.08
42	n-Nonadecane <sup>#</sup>	603.0	0.789	268.5	56.03	60.44	7.88	60.20	7.45
43	Benzene <sup>#</sup>	353.1	0.885	78.1	30.49	28.68	-5.92	28.75	-5.69
45	o-Xylene <sup>#</sup>	417.0	0.885	106.2	36.51	36.16	-0.96	35.98	-1.44

47	p-Xylene <sup>#</sup>	411.5	0.866	106.2	35.76	35.59	-0.48	35.46	-0.83
48	Cyclohexane <sup>#</sup>	353.0	0.784	84.2	29.81	29.29	-1.74	29.27	-1.81
50	Cyclopentane <sup>*</sup>	322.4	0.751	70.1	27.30	26.14	-4.24	26.07	-4.51
51	Methyl cyclopentane <sup>*</sup>	345.0	0.754	84.2	29.08	28.51	-1.96	28.55	-1.83
53	cis-Butene-2 <sup>*</sup>	276.9	0.628	56.1	23.34	21.96	-5.89	21.81	-6.55
54	Ethyl benzene <sup>*</sup>	409.3	0.872	106.2	35.57	35.22	-0.97	35.17	-1.13
55	n-Heneicosane <sup>δ</sup>	629.7	0.795	296.6	66.08	63.94	-3.24	63.75	-3.52
57	n-Tricosane <sup>δ</sup>	653.3	0.801	324.6	69.51	67.00	-3.61	66.92	-3.73
58	n-Tetracosane <sup>δ</sup>	664.5	0.803	338.7	71.16	68.48	-3.77	68.44	-3.82
60	n-Hexacosane <sup>δ</sup>	685.4	0.807	366.7	74.31	71.22	-4.16	71.31	-4.04
62	n-Octacosane <sup>δ</sup>	704.8	0.810	394.8	77.30	73.79	-4.55	74.00	-4.26
64	n-Triacontane <sup>δ</sup>	722.8	0.813	422.8	80.12	76.16	-4.94	76.52	-4.49
	<b>AARD %</b>						<b>2.75</b>		<b>2.79</b>
<b>Validation data set of Pure Hydrocarbons</b>									
2	n-Butane <sup>#</sup>	272.7	0.585	58.1	22.44	21.73	-3.19	21.60	-3.76
5	iso-Pentane <sup>#</sup>	301.0	0.625	72.2	24.69	24.42	-1.08	24.43	-1.06
11	2,3-Dimethyl butane <sup>#</sup>	321.1	0.667	86.2	27.38	26.12	-4.60	26.39	-3.60
17	2,3-Dimethyl pentane <sup>#</sup>	362.9	0.700	100.2	30.46	30.87	1.35	30.90	1.46
23	3-Methyl heptane <sup>#</sup>	392.1	0.711	114.2	33.66	34.30	1.90	34.22	1.67
25	3-Ethylhexane <sup>#</sup>	391.7	0.718	114.2	33.59	34.16	1.70	34.13	1.60
27	2,3-Dimethyl hexane <sup>#</sup>	388.8	0.717	114.2	33.17	33.77	1.80	33.79	1.88
31	3,4-Dimethyl hexane <sup>#</sup>	390.9	0.724	114.2	33.24	33.98	2.22	33.99	2.26
35	2,2,4-Trimethyl pentane <sup>#</sup>	372.4	0.697	114.2	30.79	31.73	3.06	32.02	4.00
39	n-Decane <sup>#</sup>	447.0	0.735	142.3	38.95	40.93	5.09	40.64	4.33
41	n-Octadecane <sup>#</sup>	590.0	0.786	254.5	54.37	58.78	8.11	58.49	7.58
44	Toluene <sup>#</sup>	383.8	0.872	92.1	33.17	32.29	-2.64	32.25	-2.78
46	m-Xylene <sup>#</sup>	412.3	0.869	106.2	36.11	35.67	-1.22	35.54	-1.59
49	Methyl cyclohexane <sup>#</sup>	374.0	0.774	98.2	31.44	31.68	0.75	31.70	0.84
52	Ethyl cyclohexane <sup>*</sup>	404.9	0.793	112.2	34.04	35.22	3.47	35.16	3.29
56	n-Docosane <sup>δ</sup>	641.8	0.798	310.6	67.82	65.51	-3.41	65.37	-3.61
59	n-Pentacosane <sup>δ</sup>	675.1	0.805	352.7	72.74	69.87	-3.95	69.90	-3.91
61	n-Heptacosane <sup>δ</sup>	695.4	0.809	380.7	75.80	72.54	-4.30	72.69	-4.10
63	n-Nonacosane <sup>δ</sup>	714.0	0.812	408.8	78.73	74.99	-4.75	75.28	-4.38
	<b>AARD %</b>						<b>3.08</b>		<b>3.04</b>

<sup>#</sup>Data taken from (Gopinathan and Saraf, 2001).

<sup>\*</sup>Data obtained from (Alessandro, 1995).

<sup>δ</sup>Data obtained from (Kudchadker and Zwolinski, 1966).

**Table S2: Model Predicted Refractive Index of Pure Hydrocarbons of Training and Validation Data Set using Developed Two and Three Parameter Models (Eqns. 10 and 11) versus Experimental Values of Refractive Index**

Index of data	Hydrocarbon	T <sub>b</sub> (K)	S(-)	M (g/g-mol)	Expt. RI at 70°C	Pred. RI (-) Eqn. 10	% Error	Pred. RI (-) Eqn. 11	% Error
<b>Training data set of Pure Hydrocarbons</b>									
1	Propane	231.1	0.508	44.1	1.340	1.292	-3.59	1.286	-4.00
3	iso-Butane	261.3	0.564	58.1	1.352	1.318	-2.52	1.321	-2.32
4	n-Pentane	309.2	0.631	72.2	1.358	1.361	0.25	1.358	0.02
6	2,2-Dimethyl propane	282.7	0.597	72.2	1.319	1.329	0.74	1.340	1.58
7	n-Hexane	341.9	0.664	86.2	1.370	1.379	0.67	1.376	0.41
8	iso-Hexane	333.4	0.658	86.2	1.382	1.371	-0.76	1.373	-0.68
9	3-Methyl pentane	336.4	0.669	86.2	1.376	1.378	0.13	1.378	0.17
10	2,2-Dimethyl butane	322.9	0.655	86.2	1.369	1.364	-0.40	1.371	0.16
12	n-Heptane	371.6	0.689	100.2	1.380	1.392	0.88	1.388	0.60
13	2-Methyl hexane	363.2	0.684	100.2	1.384	1.385	0.10	1.386	0.13
14	3-Methyl hexane	365.0	0.692	100.2	1.388	1.390	0.12	1.390	0.14
15	3-Ethyl pentane	366.6	0.703	100.2	1.370	1.395	1.81	1.396	1.87
16	2,2-Dimethyl pentane	352.4	0.679	100.2	1.382	1.377	-0.36	1.383	0.10
18	2,4-Dimethyl pentane	352.4	0.678	100.2	1.381	1.377	-0.31	1.383	0.14
19	3,3-Dimethyl pentane	352.4	0.698	100.2	1.393	1.385	-0.61	1.393	0.01
20	2,2,3-Trimethyl	352.4	0.695	100.2	1.389	1.383	-0.40	1.392	0.19
21	n-Octane	398.8	0.707	114.2	1.400	1.402	0.11	1.397	-0.20
22	2-Methyl heptane	390.8	0.703	114.2	1.395	1.396	0.05	1.395	0.02
24	4-Methyl heptane	390.9	0.709	114.2	1.398	1.398	0.00	1.398	0.02
26	2,2-Dimethyl hexane	382.0	0.700	114.2	1.393	1.390	-0.24	1.394	0.06
28	2,4-Dimethyl hexane	382.6	0.705	114.2	1.395	1.392	-0.22	1.396	0.10
29	2,5-Dimethyl hexane	382.3	0.698	114.2	1.392	1.389	-0.21	1.393	0.06
30	3,3-Dimethyl hexane	385.1	0.715	114.2	1.392	1.397	0.37	1.401	0.67
32	3-Ethyl-2-methyl pentane	388.8	0.724	114.2	1.403	1.403	-0.02	1.406	0.20
33	3-Ethyl-3-methyl pentane	391.4	0.732	114.2	1.402	1.407	0.36	1.410	0.55
34	2,2,3-Trimethyl pentane	383.0	0.721	114.2	1.380	1.398	1.33	1.404	1.77
36	2,3,3-Trimethyl pentane	387.9	0.731	114.2	1.400	1.405	0.34	1.409	0.66
37	2,3,4-Trimethyl pentane	386.6	0.724	114.2	1.404	1.401	-0.18	1.406	0.13
38	n-Nonane	426.5	0.722	128.3	1.405	1.410	0.37	1.404	-0.04
40	n-Dodecane	487.5	0.753	170.3	1.421	1.423	0.12	1.419	-0.14
42	n-Nonadecane	603.0	0.789	268.5	1.441	1.437	-0.30	1.435	-0.42
43	Benzene	353.1	0.885	78.1	1.501	1.476	-1.64	1.480	-1.38
45	o-Xylene	417.0	0.885	106.2	1.505	1.482	-1.55	1.479	-1.72
47	p-Xylene	411.5	0.866	106.2	1.496	1.473	-1.54	1.471	-1.63
48	Cyclohexane	353.0	0.784	84.2	1.427	1.434	0.52	1.435	0.60
50	Cyclopentane	322.4	0.751	70.1	1.400	1.421	1.47	1.420	1.42
51	Methyl cyclopentane	345.0	0.754	84.2	1.409	1.418	0.65	1.421	0.85
53	cis-Butene-2	276.9	0.628	56.1	1.320	1.361	3.13	1.357	2.81

54	Ethyl benzene	409.3	0.872	106.2	1.495	1.474	-1.43	1.474	-1.40
55	n-Heneicosane	629.7	0.795	296.6	1.444	1.438	-0.40	1.438	-0.45
57	n-Tricosane	653.3	0.801	324.6	1.445	1.439	-0.38	1.440	-0.34
58	n-Tetracosane	664.5	0.803	338.7	1.446	1.440	-0.44	1.441	-0.35
60	n-Hexacosane	685.4	0.807	366.7	1.448	1.440	-0.56	1.443	-0.37
62	n-Octacosane	704.8	0.810	394.8	1.449	1.440	-0.65	1.444	-0.35
64	n-Triacontane	722.8	0.813	422.8	1.435	1.439	0.29	1.445	0.69
	<b>AARD %</b>						<b>0.72</b>		<b>0.71</b>
<b>Validation data set of Pure Hydrocarbons</b>									
2	n-Butane	272.7	0.585	58.1	1.333	1.336	0.26	1.333	0.02
5	iso-Pentane	301.0	0.625	72.2	1.353	1.353	0.03	1.355	0.16
11	2,3-Dimethyl butane	321.1	0.667	86.2	1.375	1.367	-0.56	1.378	0.18
17	2,3-Dimethyl pentane	362.9	0.700	100.2	1.392	1.392	-0.03	1.394	0.15
23	3-Methyl heptane	392.1	0.711	114.2	1.398	1.399	0.11	1.399	0.09
25	3-Ethylhexane	391.7	0.718	114.2	1.401	1.402	0.07	1.403	0.13
27	2,3-Dimethyl hexane	388.8	0.717	114.2	1.392	1.400	0.57	1.402	0.74
31	3,4-Dimethyl hexane	390.9	0.724	114.2	1.403	1.404	0.06	1.406	0.20
35	2,2,4-Trimethyl pentane	372.4	0.697	114.2	1.391	1.383	-0.56	1.392	0.10
39	n-Decane	447.0	0.735	142.3	1.411	1.415	0.29	1.411	-0.03
41	n-Octadecane	590.0	0.786	254.5	1.439	1.436	-0.19	1.434	-0.37
44	Toluene	383.8	0.872	92.1	1.497	1.474	-1.55	1.474	-1.52
46	m-Xylene	412.3	0.869	106.2	1.497	1.474	-1.54	1.473	-1.64
49	Methyl cyclohexane	374.0	0.774	98.2	1.450	1.428	-1.54	1.430	-1.37
52	Ethyl cyclohexane	404.9	0.793	112.2	1.432	1.439	0.46	1.439	0.47
56	n-Docosane	641.8	0.798	310.6	1.444	1.439	-0.35	1.439	-0.36
59	n-Pentacosane	675.1	0.805	352.7	1.447	1.440	-0.50	1.442	-0.36
61	n-Heptacosane	695.4	0.809	380.7	1.449	1.440	-0.62	1.444	-0.38
63	n-Nonacosane	714.0	0.812	408.8	1.450	1.440	-0.71	1.445	-0.36
	<b>AARD %</b>						<b>0.53</b>		<b>0.45</b>

**Table S3: Comparison of Predicted Enthalpies of Vaporization of Pure Hydrocarbons using Different Correlations with the Experimental Heat of Vaporization Values (Training and Validation Data Set)**

Sr. No.	Hydrocarbon	Expt. $\Delta H^{vap}$ (kJ/g-mol)	%Error Model by Gopinathan & Saraf, 2001	%Error GP Model by Parhizgar <i>et al.</i> , 2013	% Error Pred. $\Delta H^{vap}$ (kJ/g-mol) Eqn. 8 of this study	% Error Pred. $\Delta H^{vap}$ (kJ/g-mol) Eqn. 9 of this study
<b>Training data set of Pure Hydrocarbons</b>						
1	Propane	19.04	-1.68	0.93	-6.48	-7.33
3	iso-Butane	21.30	0.68	-0.58	-3.89	-3.76
4	n-Pentane	25.79	0.30	1.78	-1.36	-1.93
6	2,2-Dimethyl propane	22.74	2.93	-1.63	-1.78	-0.61
7	n-Hexane	28.85	0.34	2.04	0.25	-0.37
8	iso-Hexane	27.79	1.26	1.01	0.18	0.12

9	3-Methyl pentane	28.06	1.28	0.45	0.23	0.11
10	2,2-Dimethyl butane	26.31	3.18	-1.44	0.63	1.35
12	n-Heptane	31.77	0.05	1.98	1.34	0.67
13	2-Methyl hexane	30.62	1.17	0.93	1.54	1.39
14	3-Methyl hexane	30.89	0.83	0.81	1.16	1.00
15	3-Ethyl pentane	31.12	0.56	0.28	0.72	0.61
16	2,2-Dimethyl pentane	29.23	2.44	-0.44	1.52	2.09
18	2,4-Dimethyl pentane	29.55	1.33	0.71	0.45	1.01
19	3,3-Dimethyl pentane	29.62	1.05	-0.70	-0.50	0.33
20	2,2,3-Trimethyl	28.90	3.58	-2.87	2.08	2.89
21	n-Octane	34.41	0.01	1.40	2.57	1.84
22	2-Methyl heptane	33.26	1.13	0.45	2.86	2.61
24	4-Methyl heptane	33.35	0.88	0.33	2.41	2.24
26	2,2-Dimethyl hexane	32.07	2.23	-0.59	2.96	3.27
28	2,4-Dimethyl hexane	32.51	1.01	0.29	1.64	1.98
29	2,5-Dimethyl hexane	32.54	0.84	0.90	1.67	1.93
30	3,3-Dimethyl hexane	32.31	2.37	-1.75	2.99	3.29
32	3-Ethyl-2-methyl pentane	32.93	1.52	-1.65	2.29	2.47
33	3-Ethyl-3-methyl pentane	32.78	2.74	-3.91	3.58	3.70
34	2,2,3-Trimethyl pentane	31.94	2.91	-3.01	3.06	3.59
36	2,3,3-Trimethyl pentane	32.12	3.79	-5.19	4.23	4.58
37	2,3,4-Trimethyl pentane	32.36	2.64	-2.91	3.15	3.48
38	n-Nonane	36.39	2.00	-1.48	6.04	5.10
40	n-Dodecane	43.31	-0.36	-2.22	5.76	5.08
42	n-Nonadecane	56.03	-2.06	-7.97	7.88	7.45
43	Benzene	30.49	-1.93	0.03	-5.92	-5.69
45	o-Xylene	36.51	-1.17	-2.35	-0.96	-1.44
47	p-Xylene	35.76	-0.57	-0.64	-0.48	-0.83
48	Cyclohexane	29.81	0.44	-0.24	-1.74	-1.81
50	Cyclopentane	27.30	-0.92	0.39	-4.24	-4.51
51	Methyl cyclopentane	29.08	0.39	-0.90	-1.96	-1.83
53	cis-Butene-2	23.34	-2.09	-0.14	-5.89	-6.55
54	Ethyl benzene	35.57	-0.65	-0.89	-0.97	-1.13
55	n-Heneicosane	66.08	-12.78	2.09	-3.24	-3.52
57	n-Tricosane	69.51	-13.56	1.34	-3.61	-3.73
58	n-Tetracosane	71.16	-13.93	0.99	-3.77	-3.82
60	n-Hexacosane	74.31	-14.64	0.36	-4.16	-4.04
62	n-Octacosane	77.30	-15.31	-0.20	-4.55	-4.26
64	n-Triacontane	80.12	-15.92	-0.74	-4.94	-4.49
	<b>AARD %</b>		<b>3.18</b>	<b>1.42</b>	<b>2.75</b>	<b>2.79</b>
<b>Validation data set of Pure Hydrocarbons</b>						
2	n-Butane	22.44	0.20	0.41	-3.19	-3.76
5	iso-Pentane	24.69	1.66	0.02	-1.08	-1.06

11	2,3-Dimethyl butane	27.38	-1.50	2.03	-4.60	-3.60
17	2,3-Dimethyl pentane	30.46	1.57	-0.66	1.35	1.46
23	3-Methyl heptane	33.66	0.29	0.80	1.90	1.67
25	3-Ethylhexane	33.59	0.37	0.19	1.70	1.60
27	2,3-Dimethyl hexane	33.17	0.79	-0.23	1.80	1.88
31	3,4-Dimethyl hexane	33.24	1.18	-1.21	2.22	2.26
35	2,2,4-Trimethyl pentane	30.79	3.47	-1.87	3.06	4.00
39	n-Decane	38.95	0.47	-0.98	5.09	4.33
41	n-Octadecane	54.37	-1.53	-7.63	8.11	7.58
44	Toluene	33.17	-0.94	0.11	-2.64	-2.78
46	m-Xylene	36.11	-1.32	-0.09	-1.22	-1.59
49	Methyl cyclohexane	31.44	1.67	-2.08	0.75	0.84
52	Ethyl cyclohexane	34.04	2.69	-3.58	3.47	3.29
56	n-Docosane	67.82	-13.17	1.70	-3.41	-3.61
59	n-Pentacosane	72.74	-14.28	0.66	-3.95	-3.91
61	n-Heptacosane	75.80	-14.93	0.00	-4.30	-4.10
63	n-Nonacosane	78.73	-15.62	-0.50	-4.75	-4.38
	<b>AARD %</b>		<b>4.09</b>	<b>1.30</b>	<b>3.08</b>	<b>3.04</b>

**Table S4: Predicted Heat of Vaporization of Petroleum Fractions using Developed Models in this Study versus the Experimental Heat of Vaporization Values**

Petroleum Fractions	$T_b$ (K)	S(-)	M (g/g-mol)	Expt. $\Delta H^{vap}$ (kJ/g-mol)	Pred. $\Delta H^{vap}$ (kJ/g-mol) Eqn. 8	% Error	Pred. $\Delta H^{vap}$ (kJ/g-mol) Eqn. 9	% Error
1	355.5	0.7015	95	30.80	30.03	-2.48	30.05	-2.44
2	357.2	0.7201	95	32.02	30.07	-6.09	30.12	-5.92
3	377.2	0.7321	108	33.83	32.20	-4.81	32.34	-4.41
4	377.5	0.7325	108	32.89	32.24	-1.97	32.37	-1.58
5	380.5	0.7253	107	33.95	32.77	-3.48	32.77	-3.48
6	381.1	0.7416	107	33.24	32.67	-1.71	32.73	-1.54
7	385.4	0.7534	120	36.21	32.70	-9.70	33.15	-8.46
8	402.7	0.7525	120	35.46	35.10	-1.02	35.18	-0.80
9	406.6	0.7594	120	35.29	35.56	0.78	35.59	0.84
10	407.7	0.7497	119	37.27	35.87	-3.76	35.79	-3.98
11	411.0	0.7717	134	37.09	35.58	-4.06	36.02	-2.88
12	427.4	0.7695	133	38.74	37.95	-2.04	37.99	-1.94
13	429.1	0.7709	130	38.99	38.28	-1.83	38.18	-2.07
14	431.0	0.7722	131	39.46	38.50	-2.43	38.40	-2.68
15	431.3	0.7780	133	39.16	38.40	-1.93	38.39	-1.96
16	433.3	0.7603	131	39.69	38.98	-1.79	38.77	-2.32
17	433.6	0.7739	132	39.39	38.82	-1.45	38.70	-1.75
18	434.9	0.7750	133	39.90	38.96	-2.36	38.85	-2.63

19	437.1	0.7761	139	39.14	39.06	-0.20	39.11	-0.09
20	437.4	0.7763	134	40.51	39.27	-3.07	39.14	-3.38
21	439.8	0.7777	136	40.44	39.53	-2.25	39.42	-2.52
22	443.0	0.7791	137	39.66	39.94	0.70	39.80	0.34
23	445.7	0.7805	139	41.09	40.25	-2.05	40.11	-2.38
24	446.2	0.7848	147	40.94	40.00	-2.29	40.14	-1.95
25	452.0	0.7833	147	41.40	40.86	-1.30	40.86	-1.31
26	455.4	0.7926	155	39.88	40.98	2.77	41.20	3.31
27	457.2	0.7820	146	42.74	41.67	-2.51	41.50	-2.89
28	457.3	0.7948	147	42.45	41.48	-2.28	41.41	-2.44
29	461.1	0.8143	159	41.05	41.41	0.88	41.73	1.65
30	467.6	0.8069	171	41.39	42.09	1.70	42.58	2.88
31	477.7	0.7959	162	45.13	43.98	-2.54	43.92	-2.69
32	478.3	0.8024	163	45.38	43.95	-3.15	43.94	-3.18
33	481.5	0.8136	162	45.44	44.30	-2.50	44.24	-2.64
34	490.7	0.8090	171	44.78	45.45	1.50	45.42	1.44
35	502.4	0.8526	201	51.27	45.73	-10.80	46.52	-9.26
36	503.7	0.8148	180	48.03	47.04	-2.07	47.00	-2.14
37	506.8	0.8155	180	47.82	47.49	-0.69	47.39	-0.90
38	509.2	0.8264	187	48.21	47.49	-1.50	47.60	-1.27
39	526.6	0.8293	199	49.79	49.72	-0.15	49.78	-0.03
40	530.1	0.8268	199	51.16	50.29	-1.71	50.25	-1.79
41	530.9	0.8390	205	51.63	50.05	-3.05	50.24	-2.70
42	531.7	0.8319	199	52.14	50.45	-3.23	50.40	-3.33
43	542.4	0.8365	210	52.56	51.70	-1.64	51.73	-1.57
44	556.7	0.8398	221	55.50	53.54	-3.54	53.55	-3.51
45	556.8	0.8483	226	54.97	53.28	-3.07	53.48	-2.71
46	557.4	0.8414	220	55.36	53.65	-3.09	53.63	-3.13
47	559.3	0.8482	232	53.07	53.51	0.82	53.81	1.39
48	577.7	0.8640	243	58.17	55.80	-4.07	56.05	-3.64
49	582.1	0.8558	249	58.45	56.46	-3.40	56.71	-2.98
50	583.3	0.8512	244	58.69	56.86	-3.12	56.91	-3.03
51	595.0	0.8602	256	59.71	58.22	-2.49	58.37	-2.25
52	601.2	0.8748	267	61.37	58.67	-4.40	59.04	-3.80
53	607.0	0.8700	272	62.34	59.53	-4.50	59.86	-3.98
54	610.5	0.8699	268	62.86	60.19	-4.25	60.32	-4.03
55	624.4	0.8814	295	66.37	61.52	-7.31	62.06	-6.49
56	629.6	0.8798	299	68.15	62.27	-8.62	62.78	-7.89
57	634.3	0.8786	296	69.65	63.12	-9.38	63.42	-8.94
58	646.8	0.8933	325	73.03	64.16	-12.14	64.95	-11.06
<b>AARD %</b>						<b>3.18</b>		<b>3.07</b>

Experimental heat of vaporization for petroleum fractions data taken from Fang *et al.* 2003.

**Table S5: Comparison of Predicted Heat of Vaporization of Petroleum Fractions using Earlier Published Correlations and Developed Models in this Study versus the Experimental Heat of Vaporization Values**

Petroleum Fractions	Expt. $\Delta H^{\text{vap}}$ (kJ/g-mol)	% Error Model by Gopinathan & Saraf, 2001	% Error GP Model by Parhizgar <i>et al.</i> , 2013	% Error Pred. $\Delta H^{\text{vap}}$ (kJ/g-mol) Eqn. 8 of this study	% Error Pred. $\Delta H^{\text{vap}}$ (kJ/g-mol) Eqn. 9 of this study
1	30.80	-1.86	-2.07	-2.48	-2.44
2	32.02	-5.12	2.27	-6.09	-5.92
3	33.83	-4.52	0.06	-4.81	-4.41
4	32.89	-1.71	-2.52	-1.97	-1.58
5	33.95	-3.91	2.94	-3.48	-3.48
6	33.24	-1.71	-0.54	-1.71	-1.54
7	36.21	-8.64	0.57	-9.70	-8.46
8	35.46	-1.96	-0.76	-1.02	-0.80
9	35.29	-0.42	-2.57	0.78	0.84
10	37.27	-5.41	-3.31	-3.76	-3.98
11	37.09	-4.12	1.43	-4.06	-2.88
12	38.74	-4.04	0.59	-2.04	-1.94
13	38.99	-4.23	0.67	-1.83	-2.07
14	39.46	-4.90	1.24	-2.43	-2.68
15	39.16	-4.11	-0.18	-1.93	-1.96
16	39.69	-4.86	1.09	-1.79	-2.32
17	39.39	-4.08	0.23	-1.45	-1.75
18	39.90	-4.99	1.03	-2.36	-2.63
19	39.14	-2.59	-1.57	-0.20	-0.09
20	40.51	-5.81	1.76	-3.07	-3.38
21	40.44	-5.07	0.82	-2.25	-2.52
22	39.66	-2.41	-2.07	0.70	0.34
23	41.09	-5.15	0.64	-2.05	-2.38
24	40.94	-4.69	0.07	-2.29	-1.95
25	41.40	-4.36	-0.46	-1.30	-1.31
26	39.88	0.11	-4.26	2.77	3.31
27	42.74	-6.15	1.72	-2.51	-2.89
28	42.45	-5.51	1.72	-2.28	-2.44
29	41.05	-1.40	-1.64	0.88	1.65
30	41.39	-0.63	-3.14	1.70	2.88
31	45.13	-6.62	-1.05	-2.54	-2.69
32	45.38	-7.01	2.29	-3.15	-3.18
33	45.44	-6.45	2.31	-2.50	-2.64
34	44.78	-3.01	-2.30	1.50	1.44
35	51.27	-13.06	8.50	-10.80	-9.26
36	48.03	-6.86	1.21	-2.07	-2.14
37	47.82	-5.80	-0.11	-0.69	-0.90
38	48.21	-6.08	0.58	-1.50	-1.27



39	49.79	-5.53	-1.11	-0.15	-0.03
40	51.16	-7.37	0.48	-1.71	-1.79
41	51.63	-8.07	1.54	-3.05	-2.70
42	52.14	-8.81	2.12	-3.23	-3.33
43	52.56	-7.48	0.07	-1.64	-1.57
44	55.50	-9.76	1.62	-3.54	-3.51
45	54.97	-8.88	0.75	-3.07	-2.71
46	55.36	-9.41	1.21	-3.09	-3.13
47	53.07	-5.14	-3.51	0.82	1.39
48	58.17	-10.25	0.46	-4.07	-3.64
49	58.45	-9.89	0.04	-3.40	-2.98
50	58.69	-10.05	0.17	-3.12	-3.03
51	59.71	-9.58	-1.33	-2.49	-2.25
52	61.37	-11.01	-1.20	-4.40	-3.80
53	62.34	-11.43	-0.65	-4.50	-3.98
54	62.86	-11.59	-0.71	-4.25	-4.03
55	66.37	-14.12	-0.31	-7.31	-6.49
56	68.15	-15.57	1.30	-8.62	-7.89
57	69.65	-16.68	2.47	-9.38	-8.94
58	73.03	-18.78	0.12	-12.14	-11.06
<b>AARD %</b>		<b>6.53</b>	<b>1.44</b>	<b>3.18</b>	<b>3.07</b>

Experimental heat of vaporization for petroleum fractions data taken from Fang *et al.* 2003.

**Table S6: Predicted Refractive Index of Petroleum Fractions from Developed Models in this Study versus the Experimental Values of Refractive Index**

Petroleum Fractions	T <sub>b</sub> (K)	S(-)	M (g/g-mol)	Expt. RI (-) at 70°C	Pred. RI (-) Eqn. 10 of this study	% Error	Pred. RI (-) Eqn. 11 of this study	% Error
1	355.5	0.7015	95	1.3722	1.393	1.51	1.395	1.66
2	357.2	0.7201	95	1.3760	1.401	1.82	1.404	2.05
3	377.2	0.7321	108	1.3864	1.405	1.32	1.410	1.70
4	377.5	0.7325	108	1.3994	1.405	0.40	1.410	0.77
5	380.5	0.7253	107	1.3858	1.405	1.38	1.407	1.50
6	381.1	0.7416	107	1.3888	1.411	1.63	1.415	1.86
7	385.4	0.7534	120	1.4203	1.407	-0.94	1.420	0.00
8	402.7	0.7525	120	1.3995	1.416	1.18	1.420	1.44
9	406.6	0.7594	120	1.4009	1.421	1.41	1.423	1.57
10	407.7	0.7497	119	1.4025	1.418	1.14	1.418	1.12
11	411.0	0.7717	134	1.4285	1.417	-0.84	1.429	0.01
12	427.4	0.7695	133	1.4105	1.425	1.02	1.427	1.20
13	429.1	0.7709	130	1.4112	1.429	1.23	1.428	1.20
14	431.0	0.7722	131	1.4118	1.429	1.23	1.429	1.20
15	431.3	0.778	133	1.4120	1.430	1.27	1.431	1.37
16	433.3	0.7603	131	1.4120	1.426	0.99	1.423	0.78

17	433.6	0.7739	132	1.4126	1.430	1.26	1.429	1.19
18	434.9	0.775	133	1.4132	1.431	1.23	1.430	1.19
19	437.1	0.7761	139	1.4137	1.428	0.99	1.430	1.19
20	437.4	0.7763	134	1.4139	1.432	1.25	1.431	1.18
21	439.8	0.7777	136	1.4146	1.432	1.22	1.431	1.17
22	443.0	0.7791	137	1.4153	1.433	1.26	1.432	1.17
23	445.7	0.7805	139	1.4161	1.434	1.23	1.432	1.15
24	446.2	0.7848	147	1.3980	1.430	2.27	1.434	2.61
25	452.0	0.7833	147	1.4176	1.432	1.02	1.434	1.13
26	455.4	0.7926	155	1.4219	1.432	0.69	1.438	1.13
27	457.2	0.782	146	1.4180	1.435	1.18	1.433	1.06
28	457.3	0.7948	147	1.4220	1.439	1.17	1.439	1.19
29	461.1	0.8143	159	1.4493	1.439	-0.68	1.448	-0.10
30	467.6	0.8069	171	1.4292	1.433	0.25	1.444	1.07
31	477.7	0.7959	162	1.4239	1.439	1.05	1.439	1.08
32	478.3	0.8024	163	1.4276	1.441	0.93	1.442	1.03
33	481.5	0.8136	162	1.4327	1.447	0.99	1.447	1.02
34	490.7	0.809	171	1.4312	1.444	0.89	1.445	0.98
35	502.4	0.8526	201	1.4554	1.448	-0.52	1.465	0.63
36	503.7	0.8148	180	1.4310	1.447	1.09	1.448	1.17
37	506.8	0.8155	180	1.4351	1.448	0.91	1.448	0.90
38	509.2	0.8264	187	1.4406	1.449	0.59	1.453	0.85
39	526.6	0.8293	199	1.3979	1.451	3.82	1.454	4.01
40	530.1	0.8268	199	1.4397	1.452	0.84	1.453	0.91
41	530.9	0.839	205	1.4486	1.453	0.33	1.458	0.67
42	531.7	0.8319	199	1.4461	1.454	0.56	1.455	0.62
43	542.4	0.8365	210	1.4486	1.455	0.43	1.457	0.59
44	556.7	0.8398	221	1.4481	1.456	0.58	1.458	0.71
45	556.8	0.8483	226	1.4548	1.457	0.16	1.462	0.51
46	557.4	0.8414	220	1.4515	1.458	0.43	1.459	0.53
47	559.3	0.8482	232	1.4555	1.455	0.00	1.462	0.45
48	577.7	0.864	243	1.4581	1.463	0.35	1.469	0.74
49	582.1	0.8558	249	1.4590	1.460	0.05	1.465	0.43
50	583.3	0.8512	244	1.4588	1.461	0.13	1.463	0.30
51	595.0	0.8602	256	1.4636	1.463	-0.03	1.467	0.24
52	601.2	0.8748	267	1.4660	1.466	0.00	1.473	0.50
53	607.0	0.87	272	1.4684	1.465	-0.25	1.471	0.19
54	610.5	0.8699	268	1.4692	1.467	-0.12	1.471	0.13
55	624.4	0.8814	295	1.4712	1.466	-0.32	1.476	0.33
56	629.6	0.8798	299	1.4740	1.466	-0.52	1.475	0.09
57	634.3	0.8786	296	1.4795	1.469	-0.73	1.475	-0.32
58	646.8	0.8933	325	1.4750	1.468	-0.46	1.481	0.40
<b>AARD %</b>						<b>0.89</b>		<b>0.96</b>

Experimental values of refractive index for petroleum fractions data taken from Fang *et al.* 2003.